Future Directions in Computational Fluid Dynamics

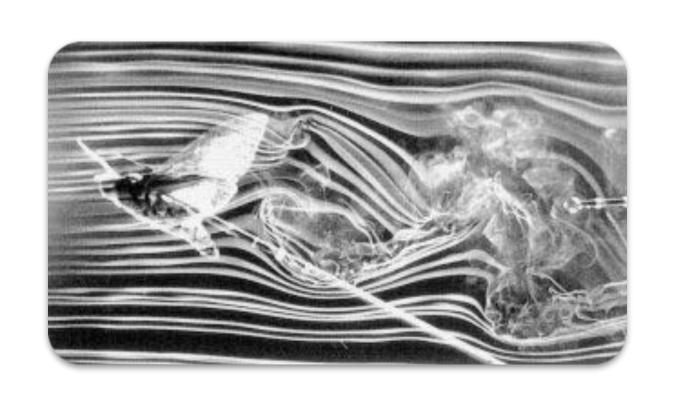
F.D. Witherden and A. Jameson

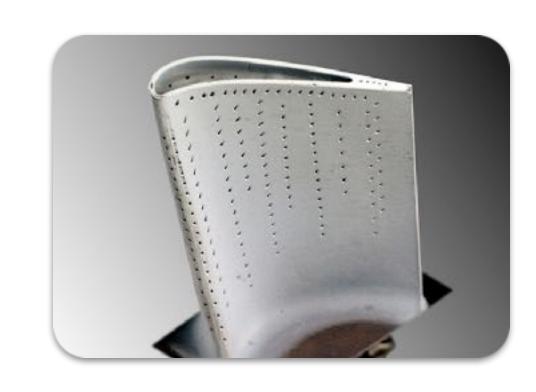
Department of Aeronautics & Astronautics
Stanford University

Why CFD?

• Since its inception CFD has been an incubator for the formulation and development of numerical algorithms.

Why is CFD Challenging?







• Three words: Shocks, separation, and turbulence.







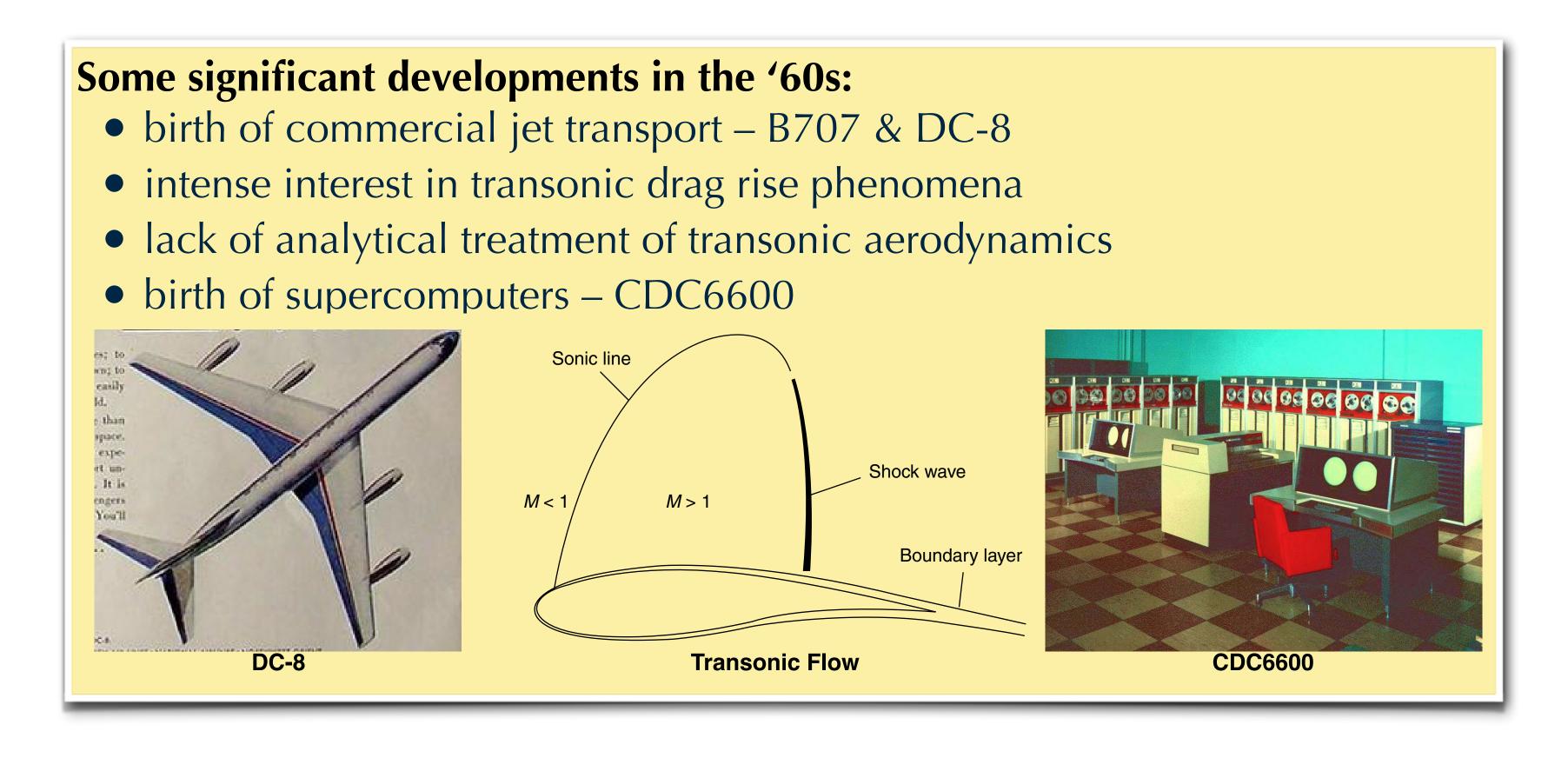
Brief History of the Evolution of CFD

Van Leer's View

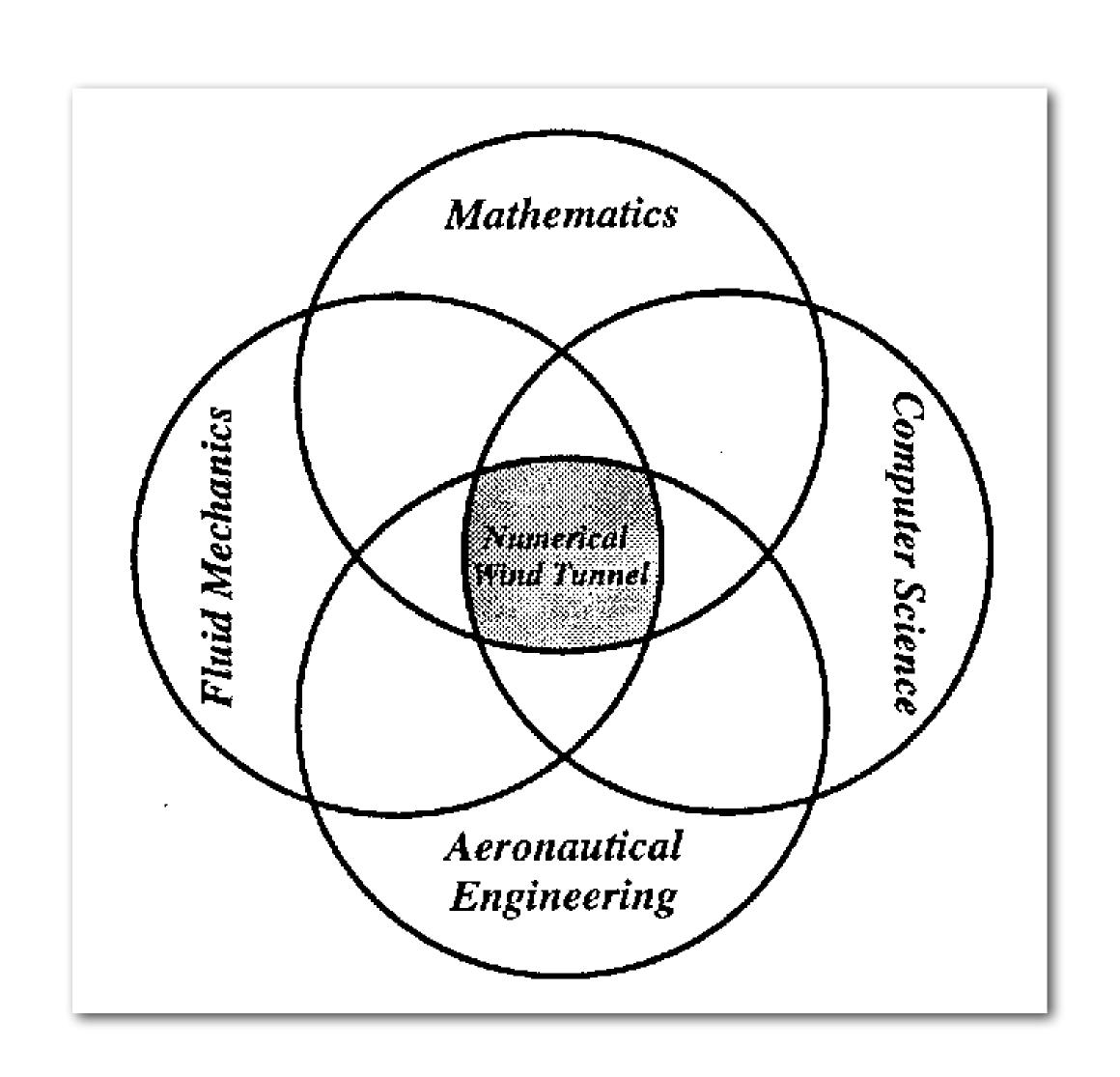


Emergence of CFD

• Driven by advances in computer power and algorithms.



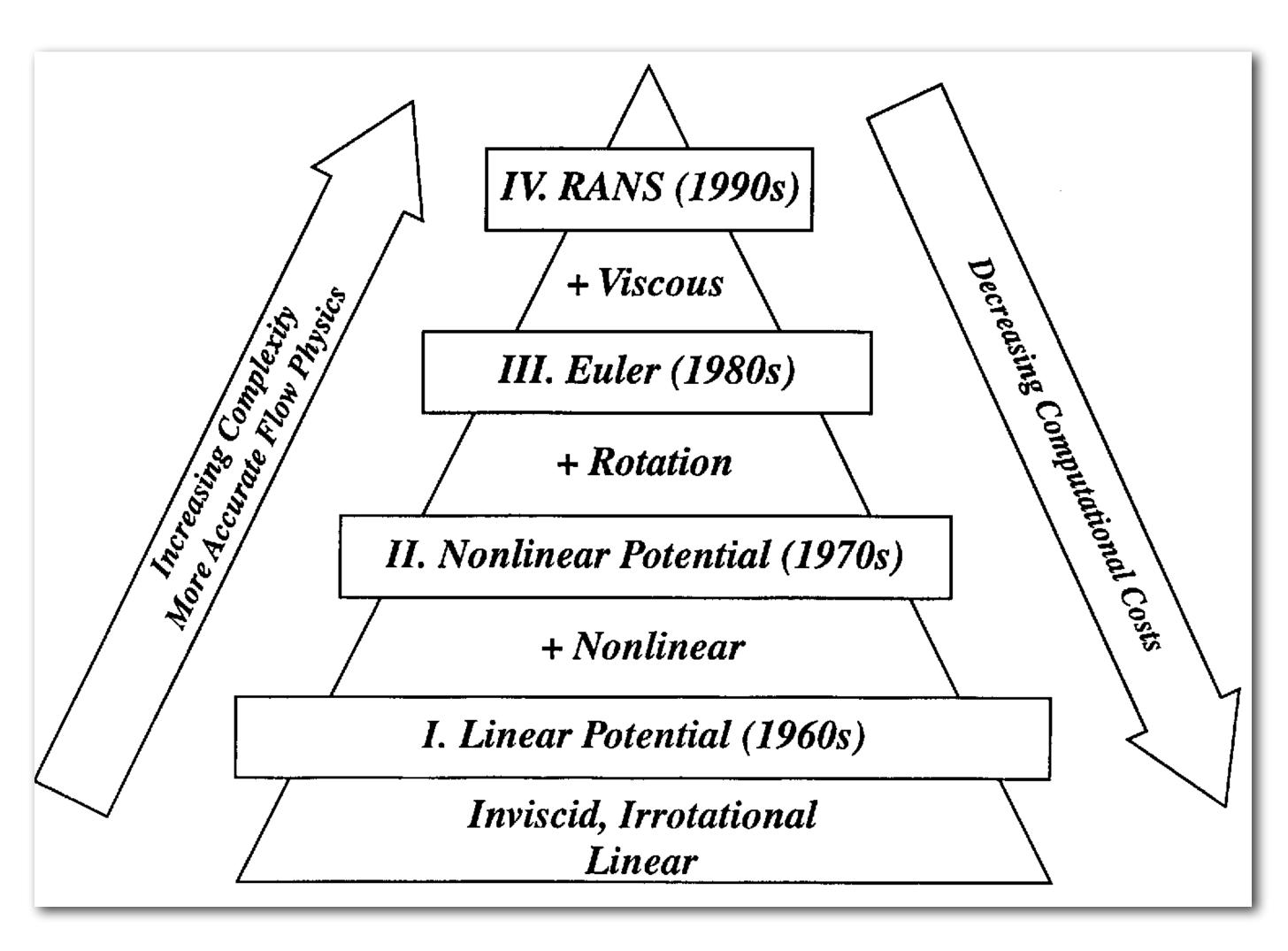
Multi-Disciplinary Nature of CFD



Advances in CFD have been paced by advances in computer power

| 1970 | CDC6600 | 1 Megaflops | 10 ⁶ |
|------|--|---------------------|-------------------------|
| 1980 | Cray 1 Vector Computer | 100 Megaflops | 10 ⁸ |
| 1994 | IBM SP2 Parallel Computer | 10 Gigaflops | 10 ¹⁰ |
| 2007 | Linux Clusters | 100 Teraflops | 10 ¹⁴ |
| 2009 | HP Pavilion Quadcore Notebook \$1,099 | 1 Gigaflops | 10 ⁹ |
| 2011 | MacBook Pro Quadcore Laptop \$2,099 | 2.5 Gigaflops 2.5×1 | |
| 2012 | Titan supercomputer @ ORNL 18,688 × NVIDIA K20 GPUs | 20 Petaflops | 2×10 ¹⁶ |

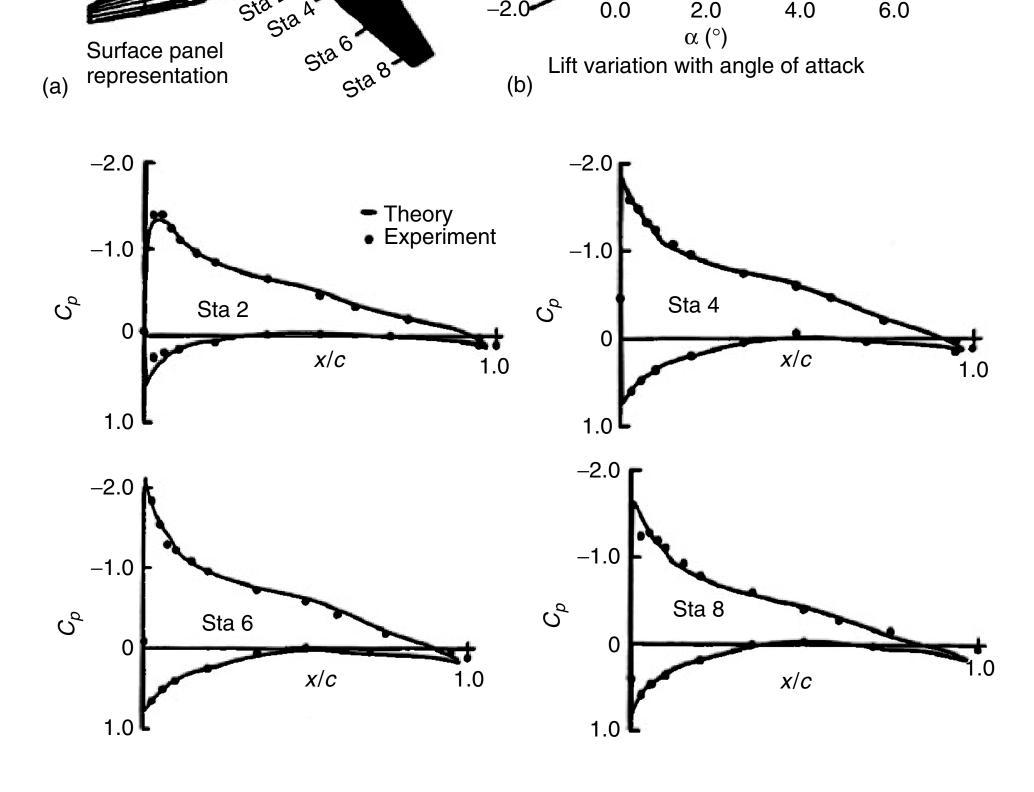
Hierarchy of Governing Equations



Panel Codes for Potential Flow

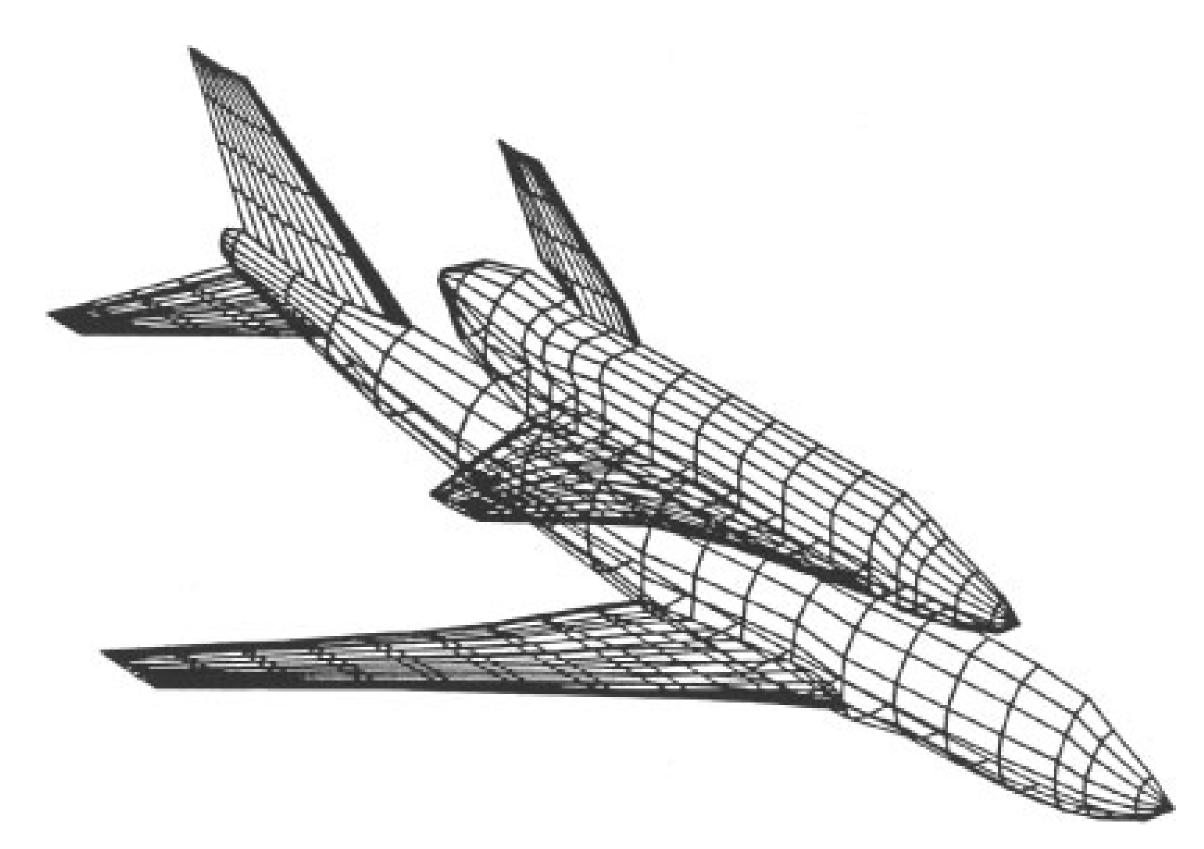
(Circa 1970)

Panel method applied to a Boeing 747. (Supplied by Paul Rubbert, the Boeing Company.)

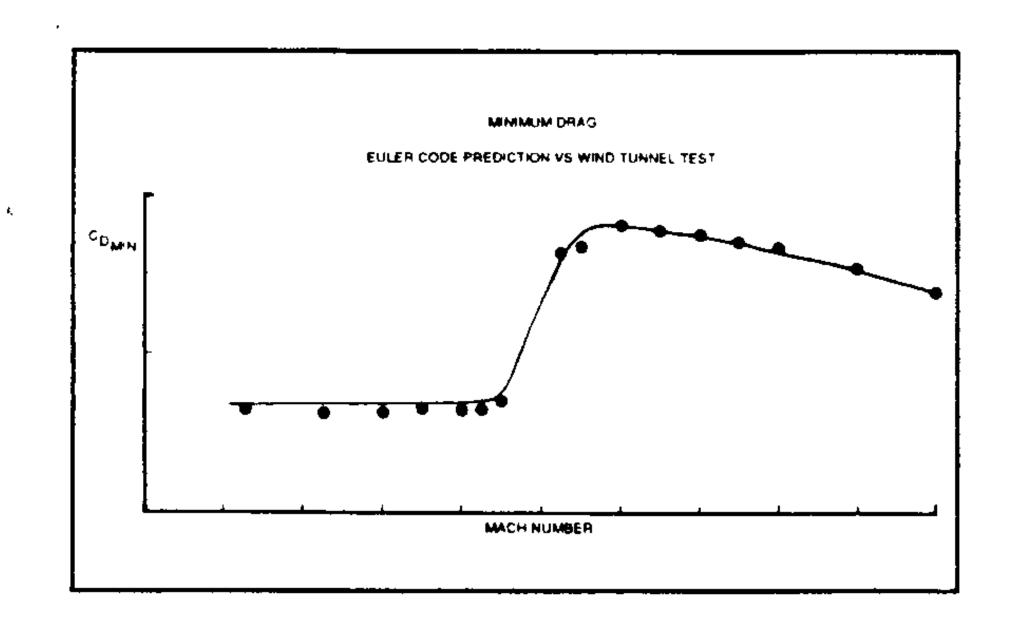


Panel Codes for Potential Flow (Circa 1970)

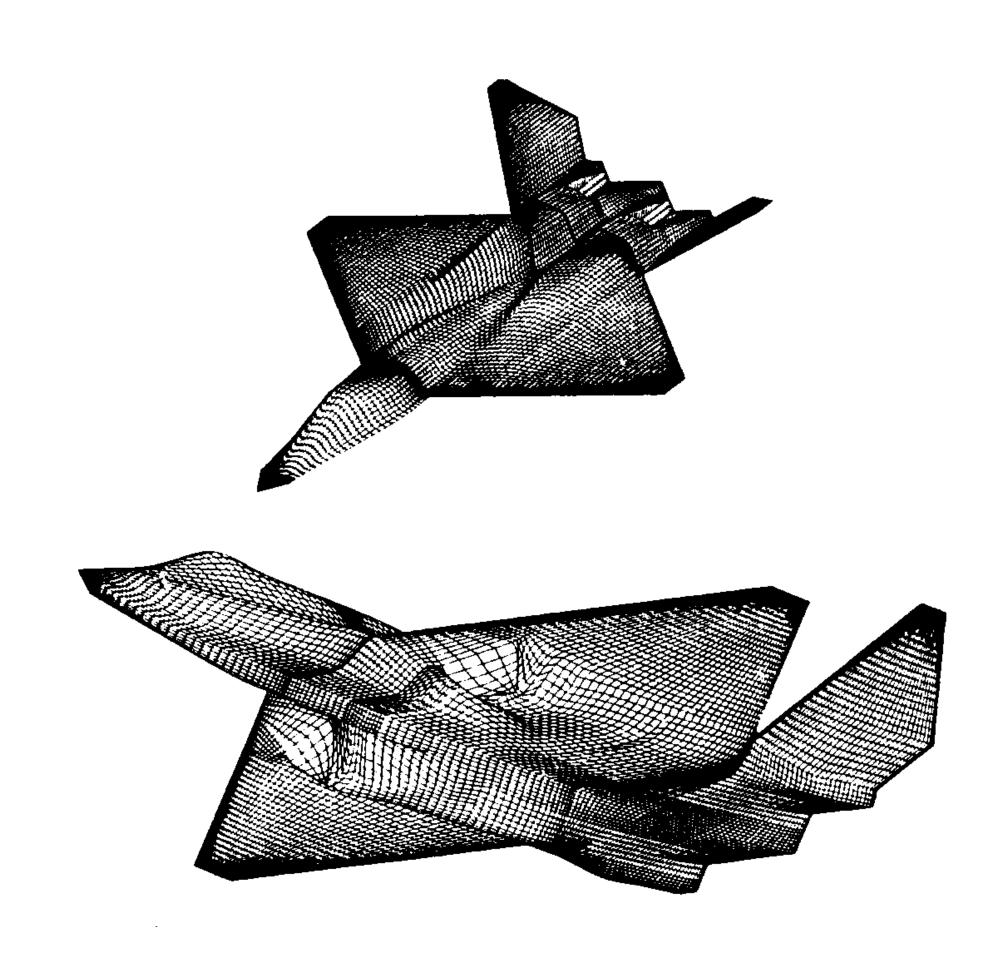
Panel method applied to flow around Boeing 747 and space shuttle. Supplied by Allen Chen, the Boeing Company.



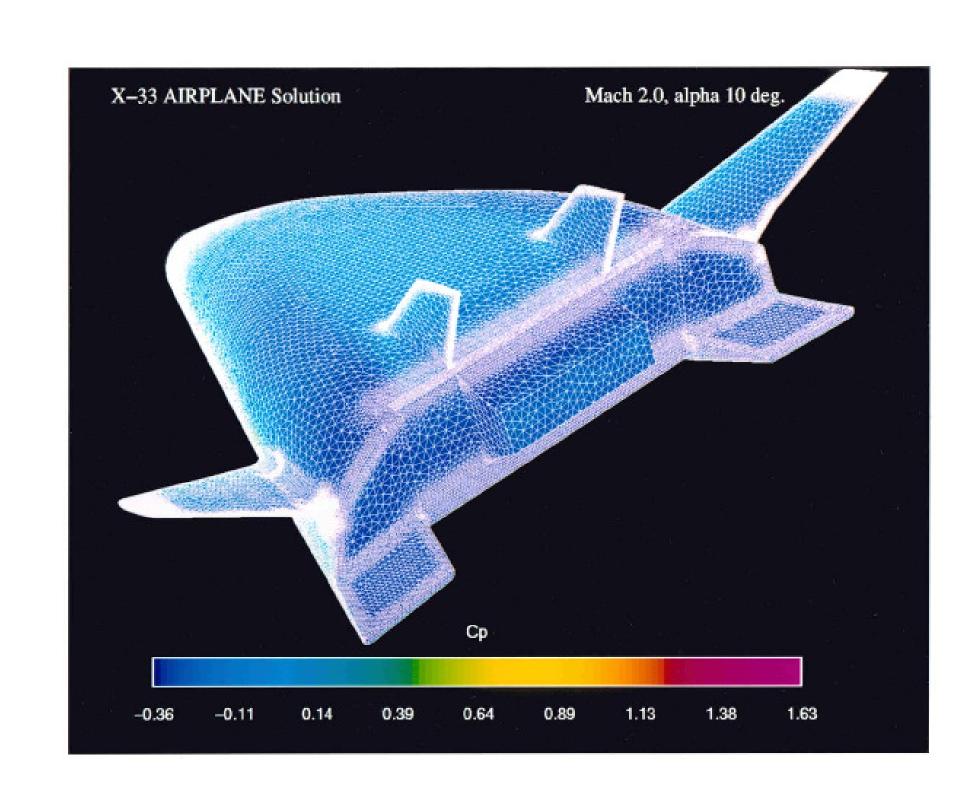
Euler Solutions (1985–1990)

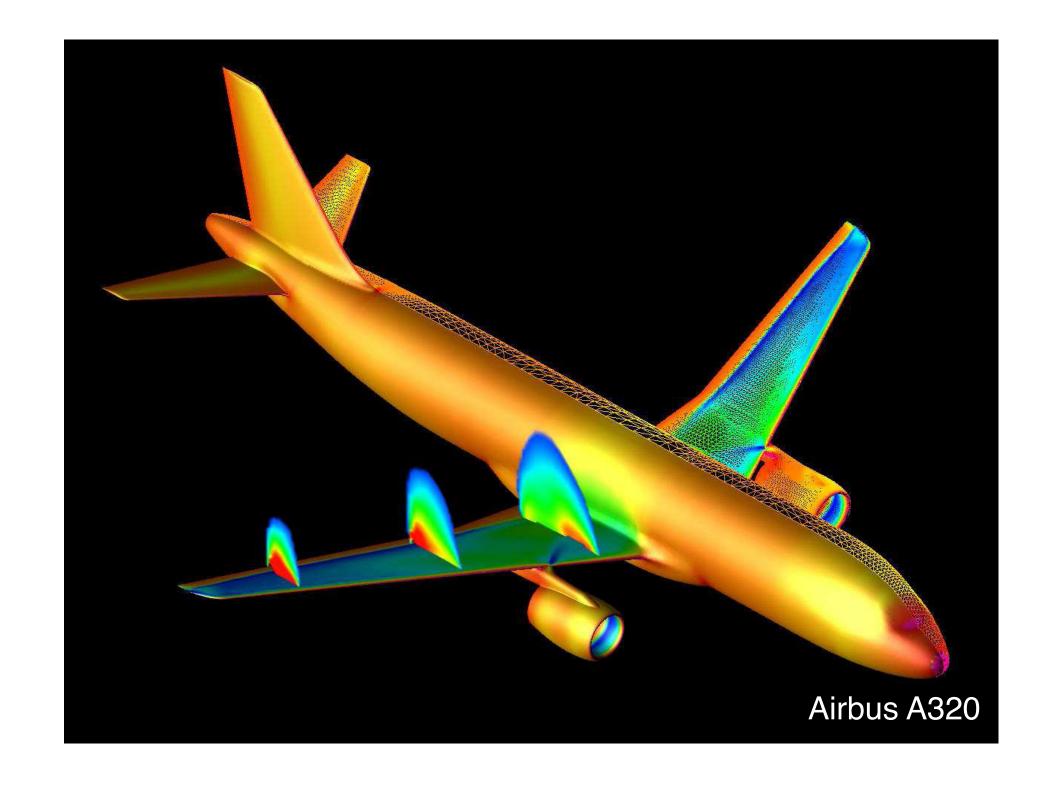


Northrop YF-23 Extended version of FLO57 by Richard Busch, Jr.

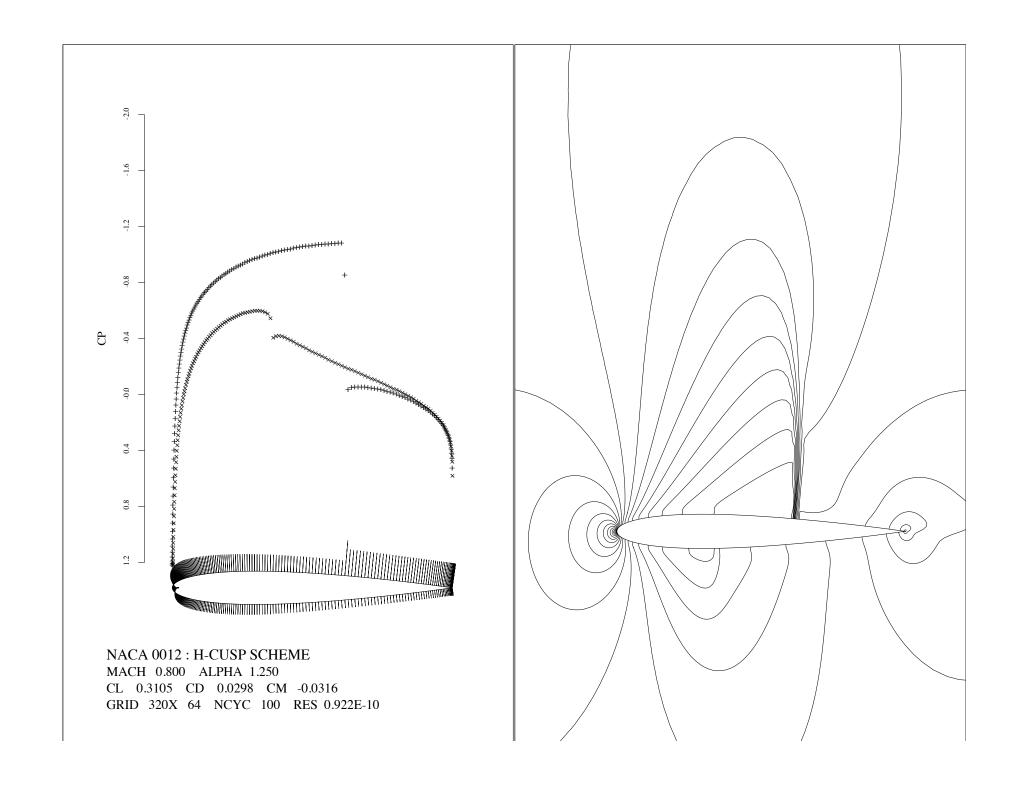


Euler Solutions (1985–1990)

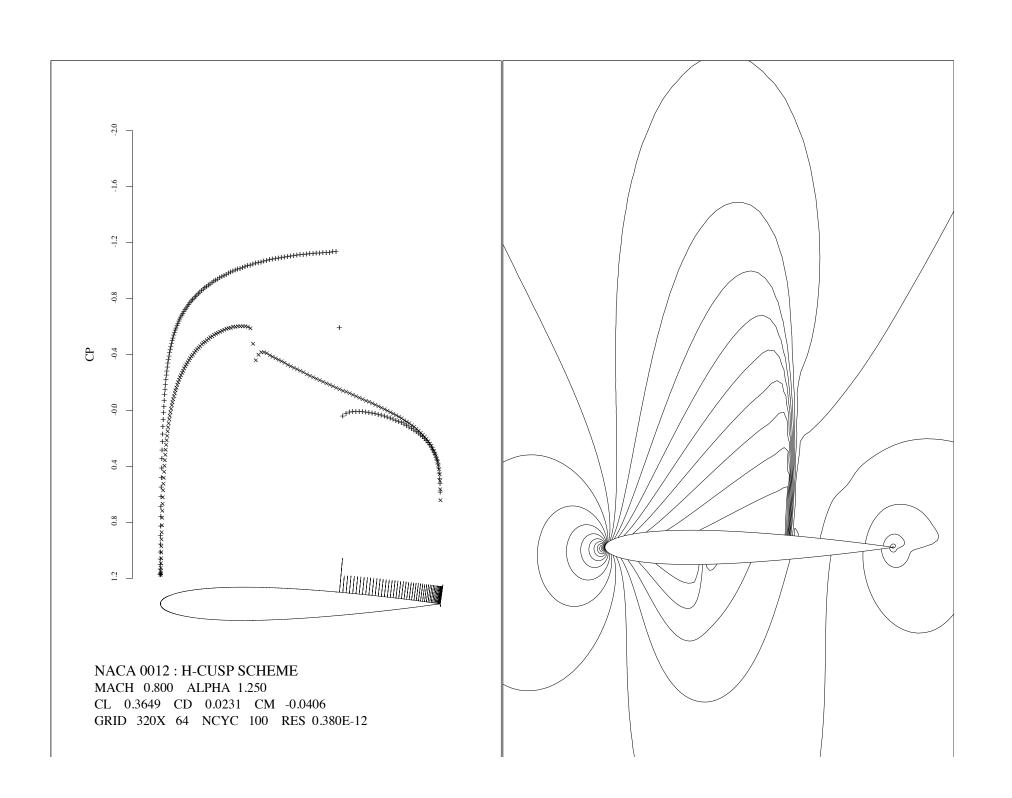




First and Second Order Accuracy



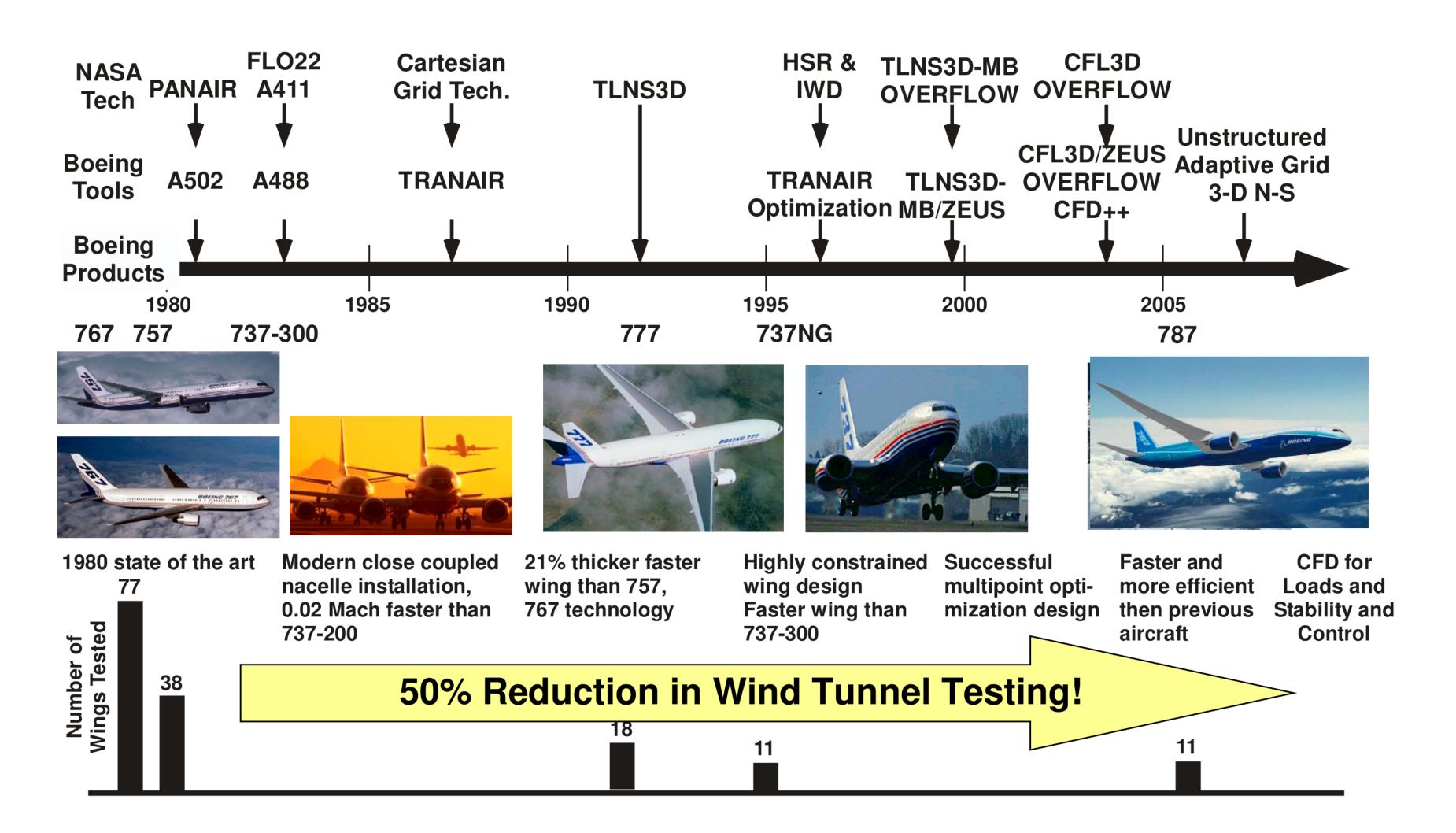
First order



Second order

Industrial Use of CFD in Aerospace

Impact of CFD at Boeing



Uses of CFD for the B787



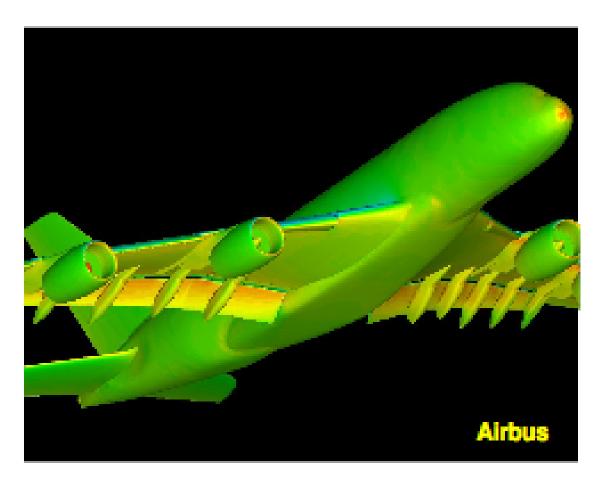
CFD at Airbus

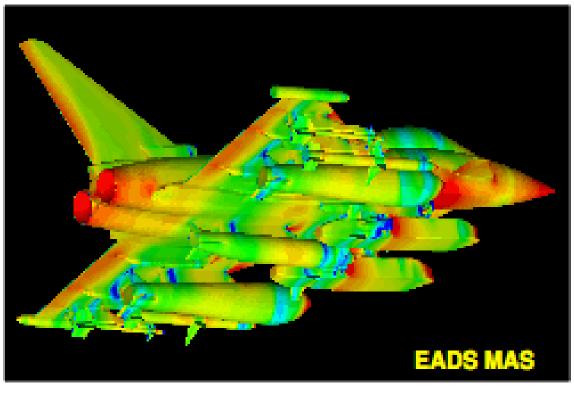
MEGAFLOW / MEGADESIGN

- National CFD Initiative (since 1995)

Development & validation of a national CFD software for complete aircraft applications which

- allows computational aerodynamic analysis for 3D complex configurations at cruise, high-lift & off-design conditions
- builds the basis for shape optimization and multidisciplinary simulation
- establishes numerical flow simulation as a routinely used tool at DLR and in German aircraft industry
- serves as a development platform for universities

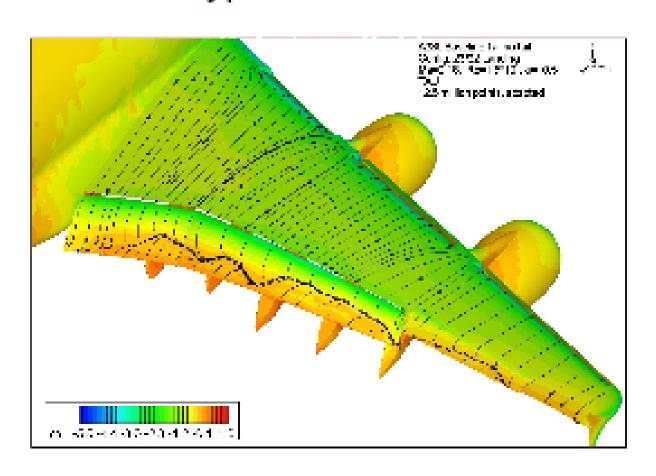


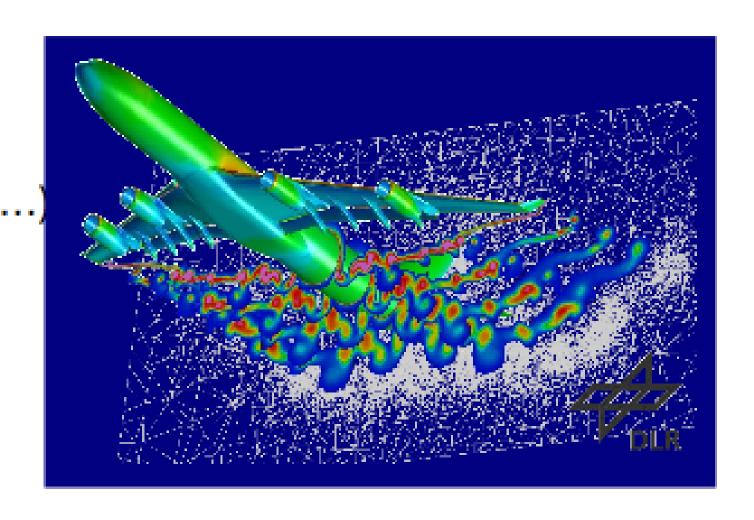


CFD at Airbus

Tool for complex configurations

- hybrid meshes, cell vertex / cell centered
- high-level turbulence & transition models (RSM, DES, linear stability methods)
- state-of-the-art algorithms (JST, multigrid, ...)
- local mesh adaptation
- chimera technique
- fluid / structure coupling
- continuous/discrete adjoint
- extensions to hypersonic flows





TAU-Code

- unstructured database
- C-code, Python
- portable code, optimized for cache hardware
- high performance on parallel computer

Uses of CFD for the A380

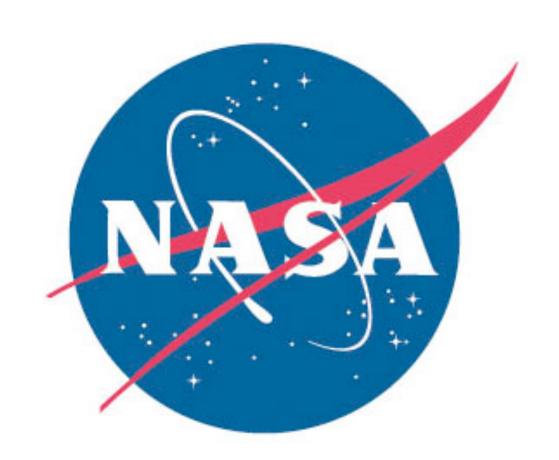


Current Status of CFD

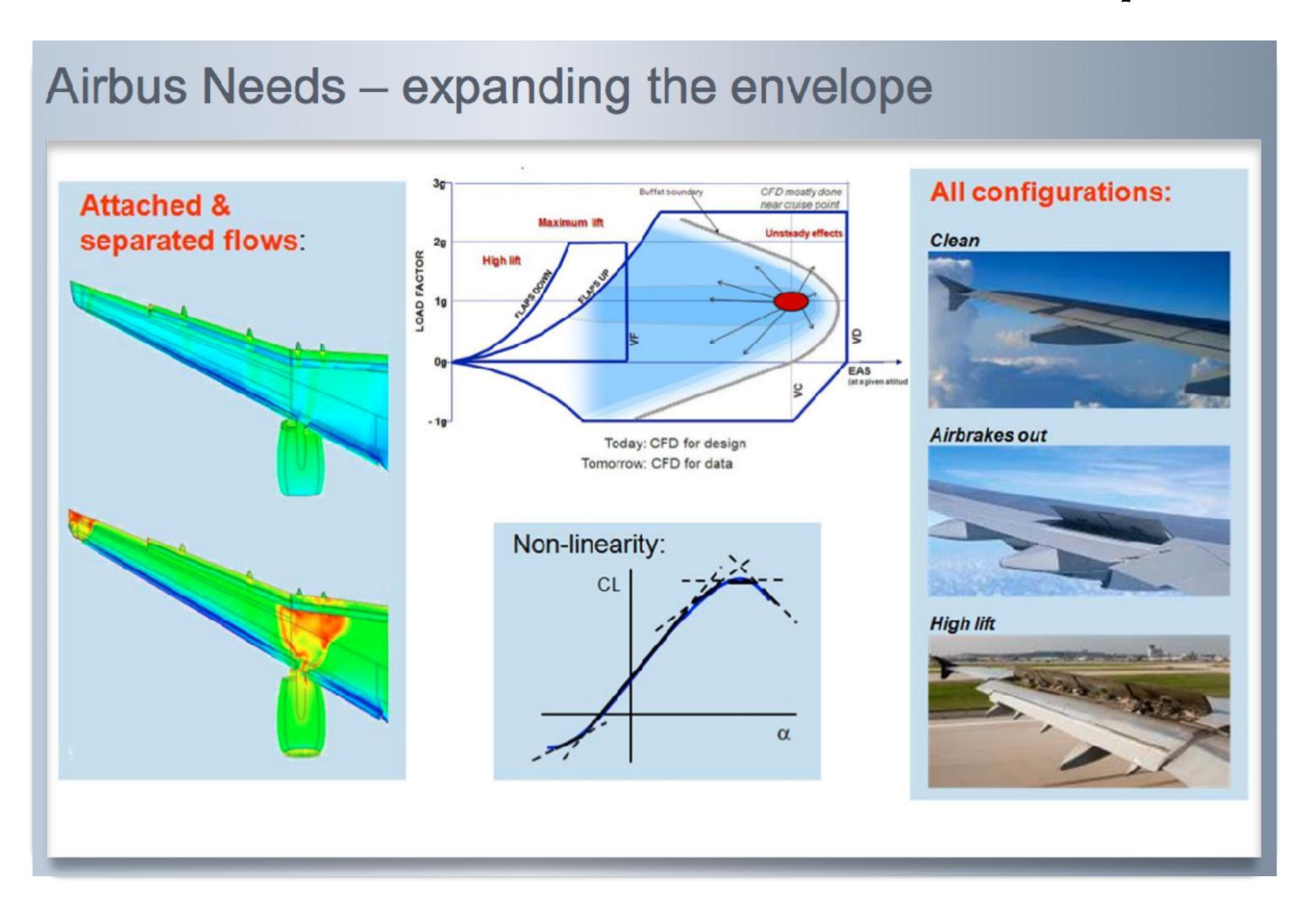
- Worldwide commercial and government codes are based on algorithms developed in the '80s and '90s
- These codes can handle complex geometry but are generally limited to 2nd order accuracy
- They cannot handle turbulence without modeling

- CFD has been on a plateau for the past 15 years
- The majority of current CFD methods are not adequate for vortex dominated and transitional flows
 - Rotorcraft, High-lift systems, Formation flying, ...

"In spite of considerable successes, reliable use of CFD has remained confined to a small but important region of the operating design space due to the inability of current methods to reliably predict turbulent-separated flows"



—NASA CFD Vision 2030 Study, 2014.



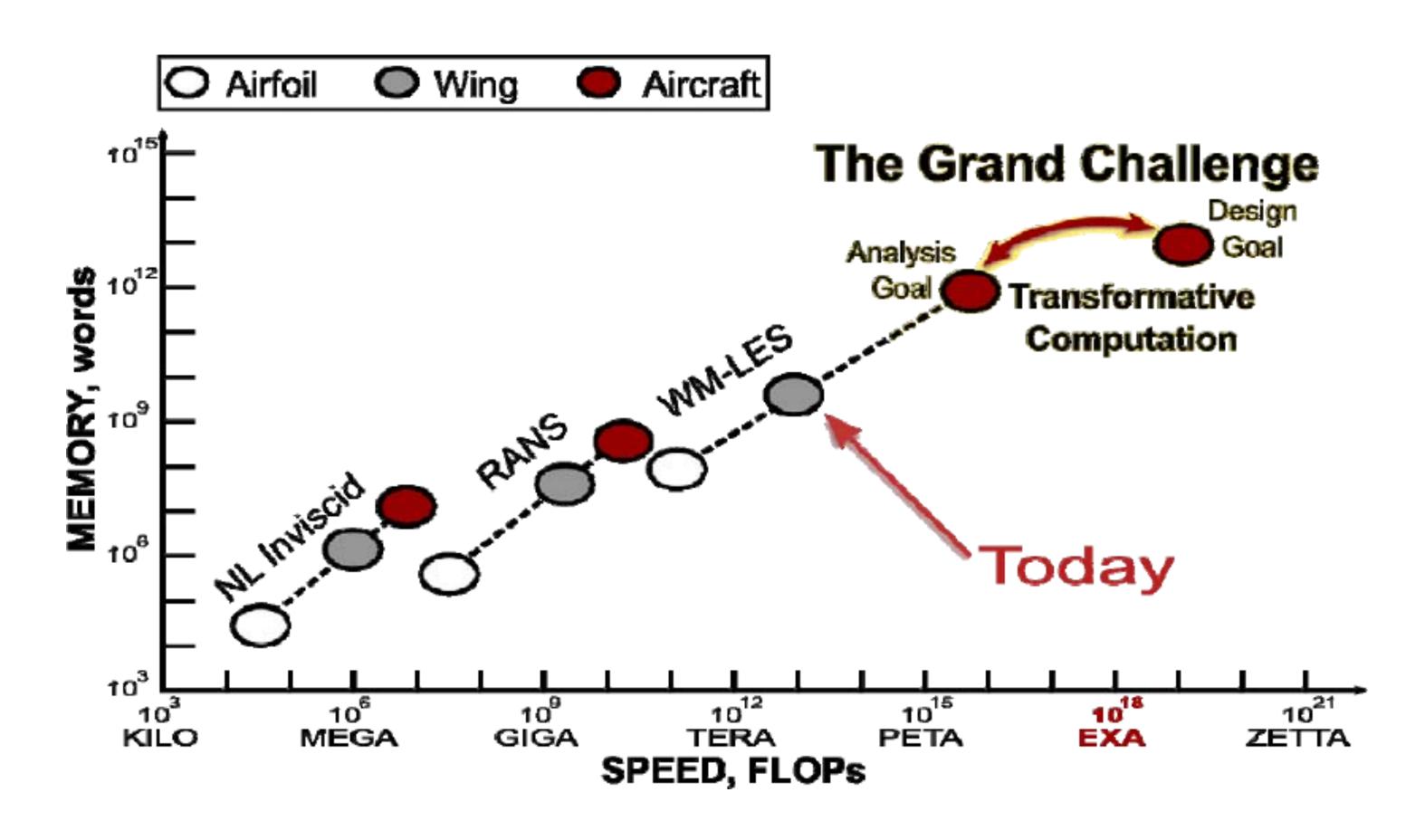
Murray Cross, Airbus, Technology Product Leader — Future Simulations (2012)

CFD in the Future

CFD Tomorrow

- To facilitate a step-change in design capabilities we need to move away from RANS simulations to large eddy simulations (LES).
- The number of DOFs for an LES of turbulent flow over an airfoil scales as Re^{1.9~2.4} (resp. Re^{0.28~0.4}) if the inner layer is resolved (resp. modeled)

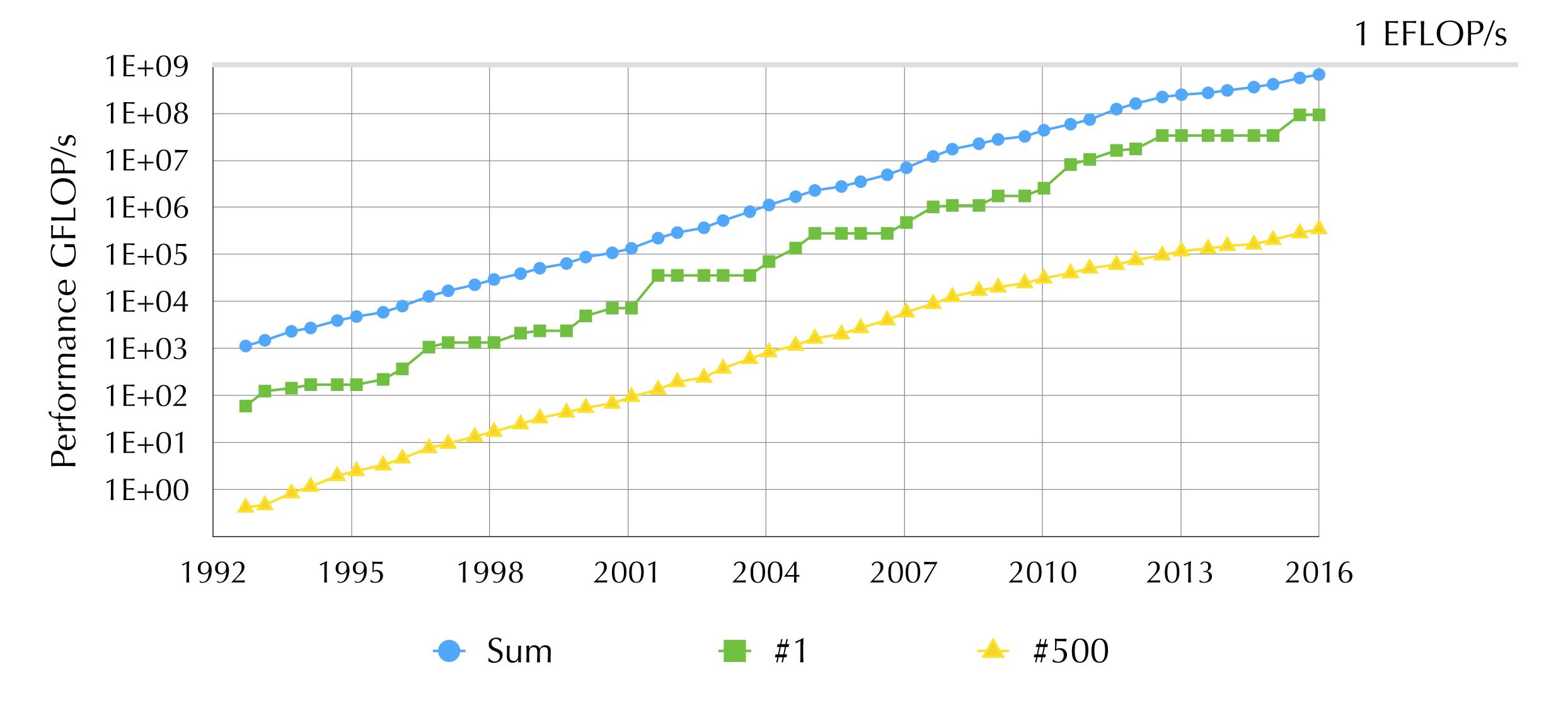
The Cost of LES



From The Opportunities and Challenges of Exascale Computing, US DOE, fall 2010.

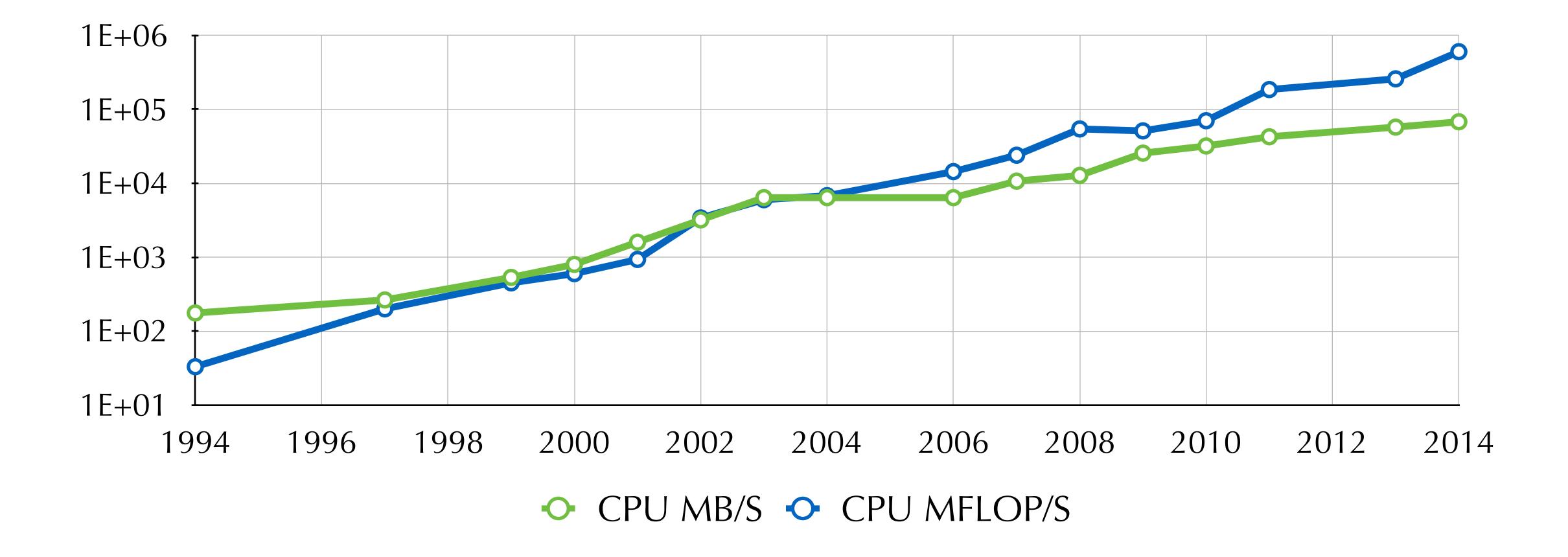
Hardware Developments

The TOP500 List



FLOP/s and Memory

• Intel server CPUs from 1994–2014...



FLOP/s and Memory

• Twenty years of progress.

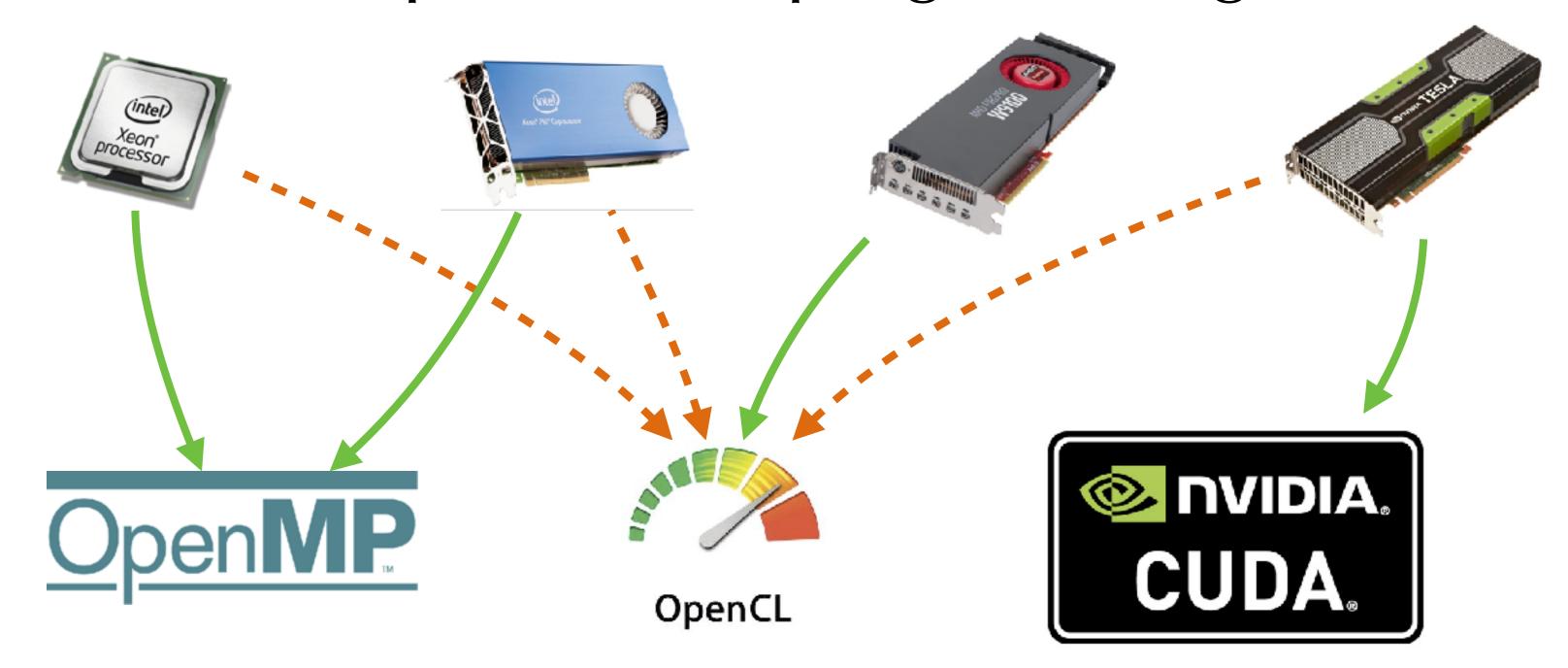
| | 1994 | 2014 | Ratio |
|---------|------|---------|--------|
| | | | |
| MFLOP/s | 33 | 604,000 | 18,303 |
| | | | |
| MB/s | 176 | 68,000 | 386 |

FLOP/s and Memory

On account of this changing landscape we need to completely rethink how we design methods now that data movement is expensive and arithmetic is cheap.

Accelerators

Accelerators complicate the programming environment.



However, they do not change the fundamentals.

Accelerators to the rescue?

- ...but they do offer tremendous FLOP rates.
- Titan at ORNL: 17.6 PFLOP/s with 18,688 K20X GPUs.



Beyond Hardware: Algorithms

- Our challenges do not stop there...
- Not only are the majority of current numerical methods ill-suited to modern hardware they are also overly dissipative.

Baseline Requirements

- A good numerical scheme for future CFD needs to:
 - have minimal dissipation
 - conserve memory bandwidth
 - permit complex geometries

High-Order Methods

For turbulent compressible flows the most promising candidates are high-order discontinuous spectral element schemes.

• Reason: High arithmetic intensity at p = 4 and above.

High-Order Methods

- Paired with **explicit time-stepping** they admit a very efficient implementation.
- Are currently enabling LES of hitherto intractable flow problems.
- However, as a community we are still far away from LES of a complete air vehicle.

Challenge I: Time-Stepping

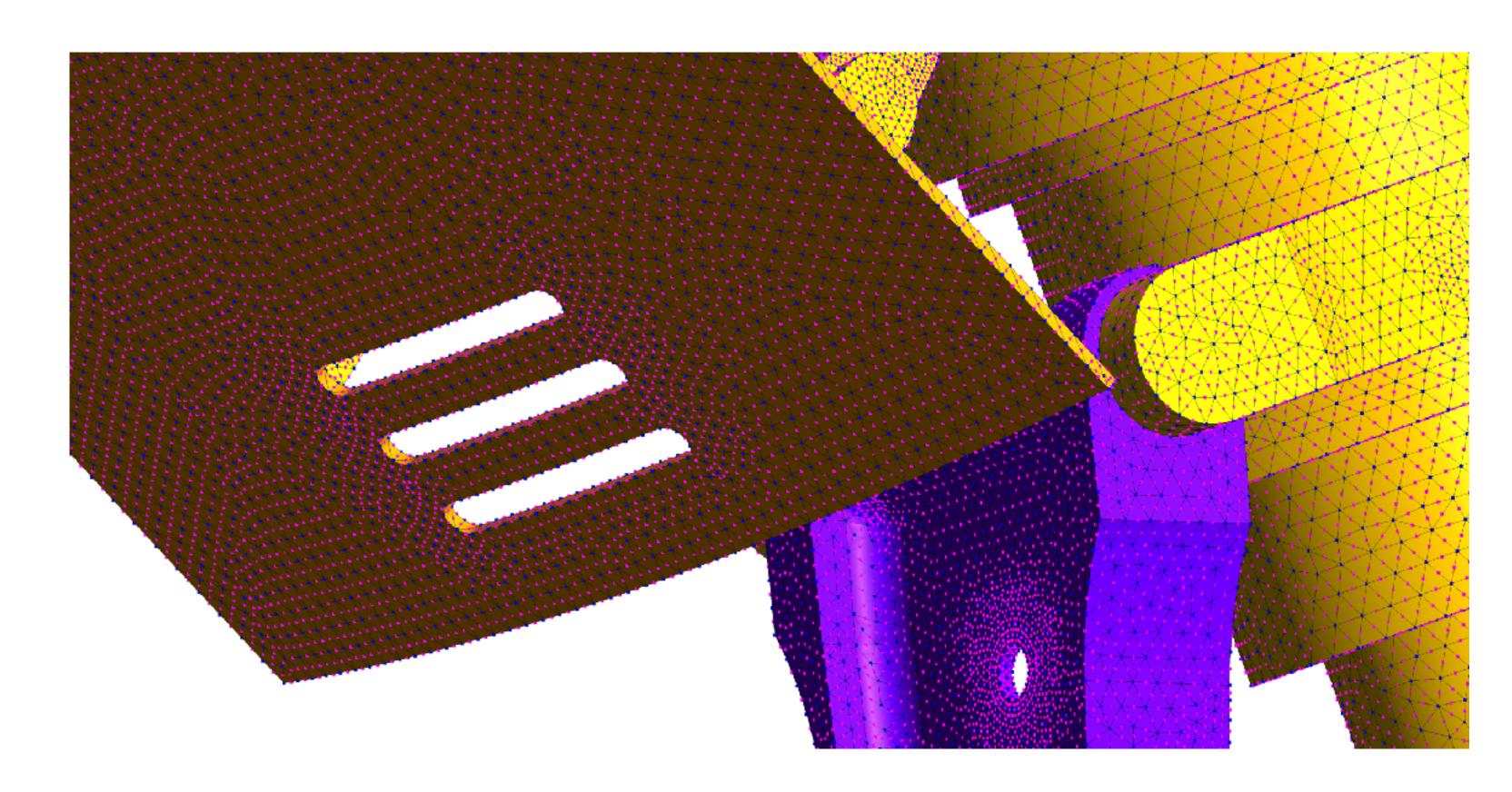
- Re > 10⁶ requires high aspect ratio near-wall grids.
- ...which necessitates implicit time-stepping.
- Existing approaches are **memory intensive** ($J \sim p^6$) and/or require pre-conditioners which are ill-suited to modern hardware.

Challenge II: Wall and Sub-grid Scale Models

- Wall models are still at an early stage.
- High-order sub-grid scale models also lacking.
- Still derived on an 'incompressible first' basis.
- Often introduce extra free parameters.

Challenge III: Grid Generation

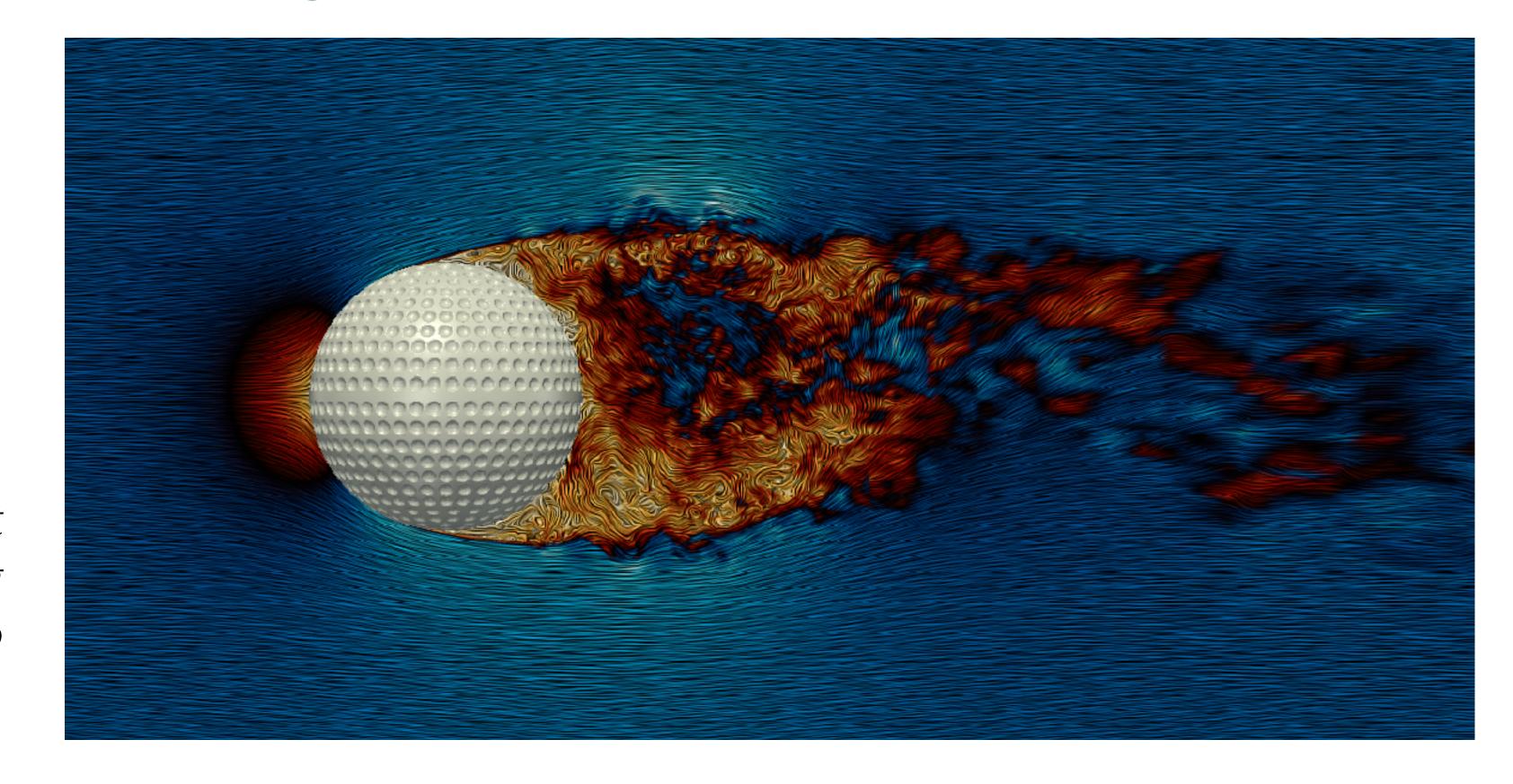
Curved body fitted grids are hard to generate.



Courtesy Steve Karman of Pointwise

Real World Flows

LES alone is not enough.



LES of a golf ball at $Re = 180 \times 10^{3} \text{ using}$ an overset grid to enable the ball to spin

Challenge IV: Dynamic Grids

- Lack efficient approaches for grid deformation.
- Also need accurate methods for high-order interpolation in overset settings.
- Some problems also require AMR.

Challenge V: FSI

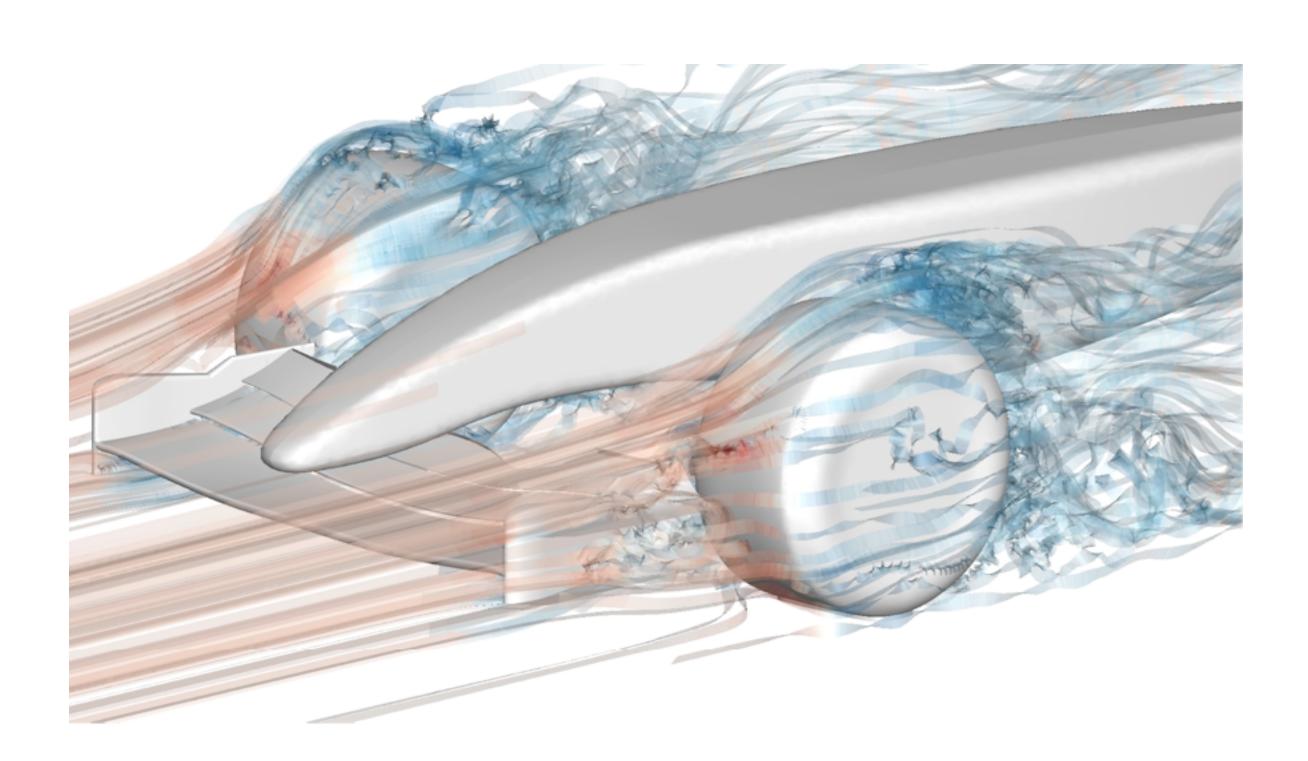
- Often Error(RANS) ~ Error(lack of structural effects)
- Thus need LES + FSI.
- But FSI = Deforming grids + solid mechanics.

Challenge VI: Multiphysics

- Requires complex sub grid scale chemical models.
- ΔT (chemistry) $\ll \Delta T$ (fluid), truly multi-scale.
- Vital for hypersonic applications.



Beyond Aerospace

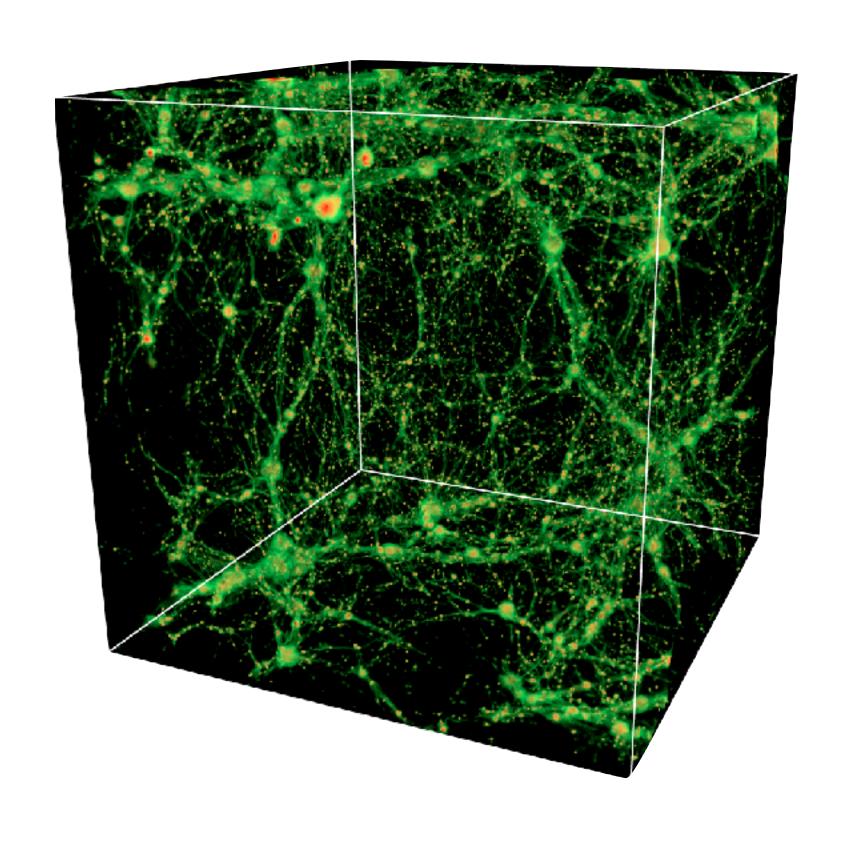




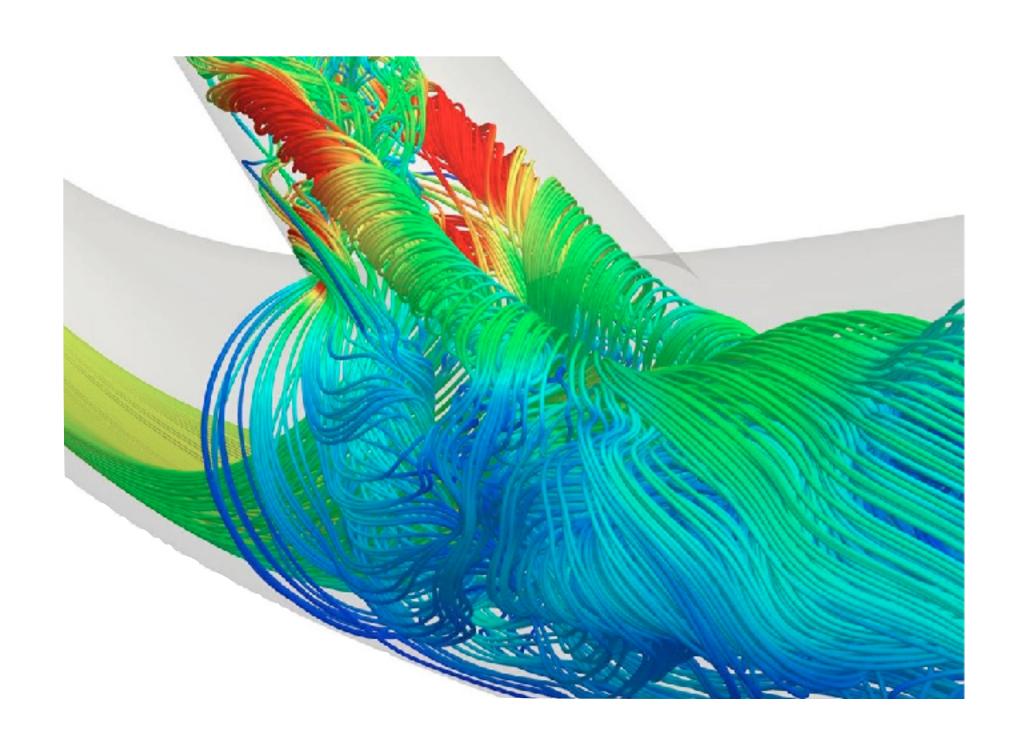
Automotive Courtesy of S. Sherwin

Marine

Beyond Aerospace



Cosmological flows From SDSC (Tiger simulation)



Bioflows

Courtesy of P. Vincent

What We're Doing

PyFR

- Flux reconstruction code designed from the ground up for modern hardware.
- Written in Python just 8,000 lines of code.
- Computational kernels specified in a Mako-derived domain specific language to enable heterogeneous computing.

PyFR

Features.

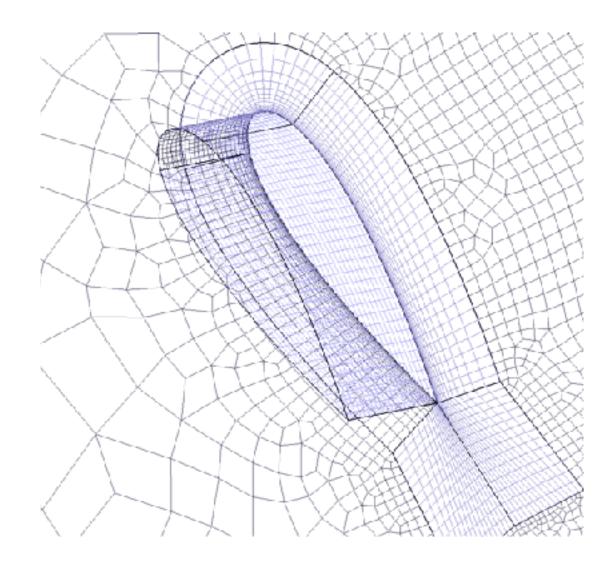
| Compressible Euler and Navier Stokes |
|--|
| Arbitrary order Flux Reconstruction on mixed unstructured grids (tris, quads, hexes, tets, prisms, and pyramids) |
| Adaptive explicit Runge-Kutta schemes |
| single double |
| None |
| CPU and Xeon Phi clusters NVIDIA GPU clusters AMD GPU clusters |
| |

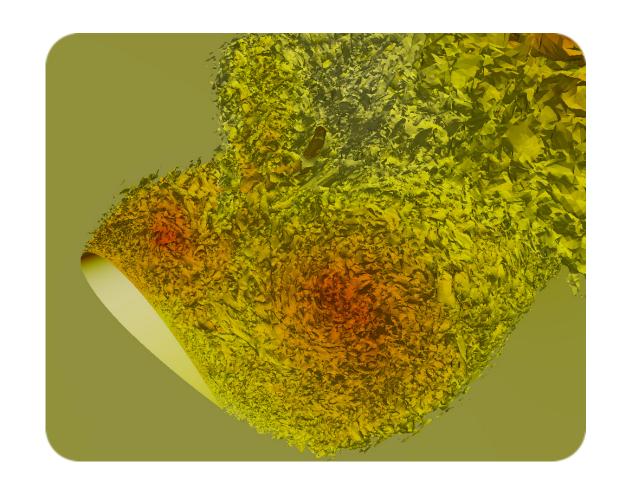
PyFR: NACA 0021

Flow over a NACA 0021 at 60 degree AoA



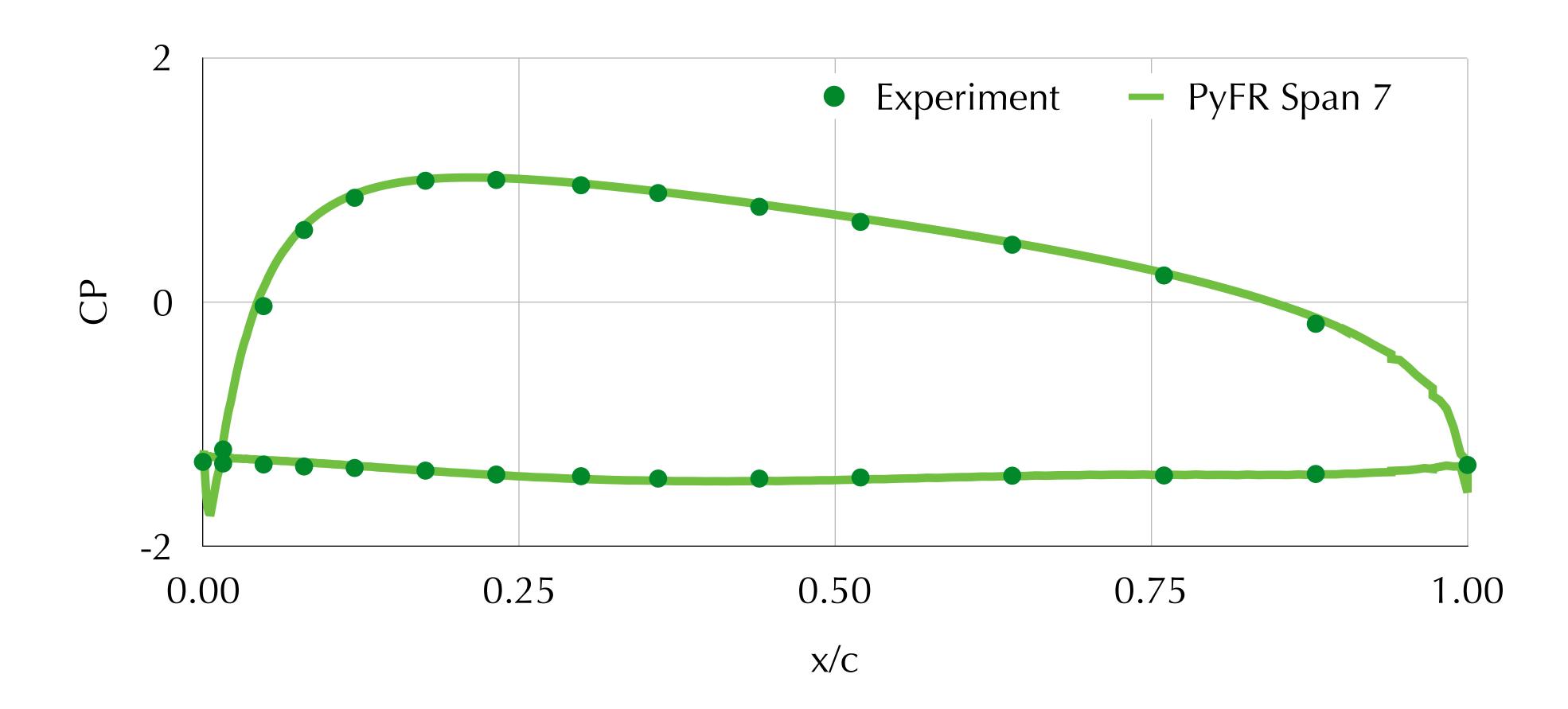
 Compare with Swalwell and DESider





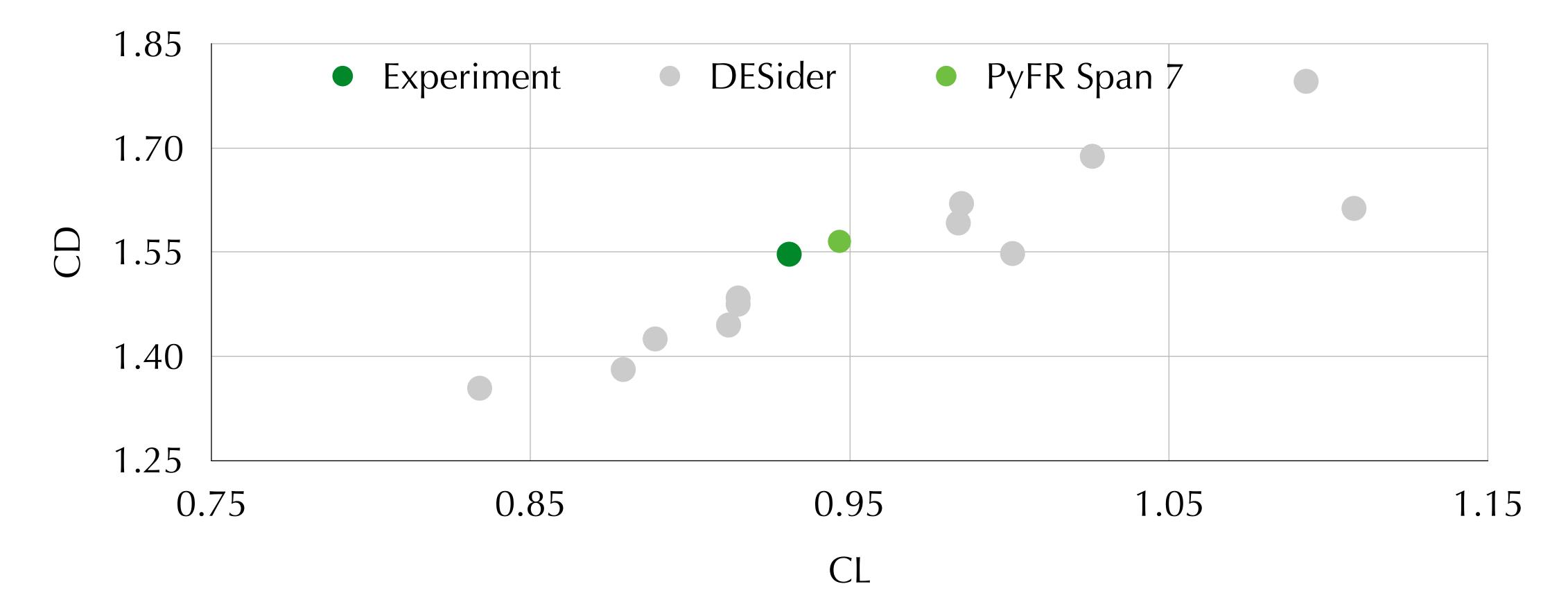
PyFR: NACA 0021

• Time-span averaged surface pressure.



PyFR: NACA 0021

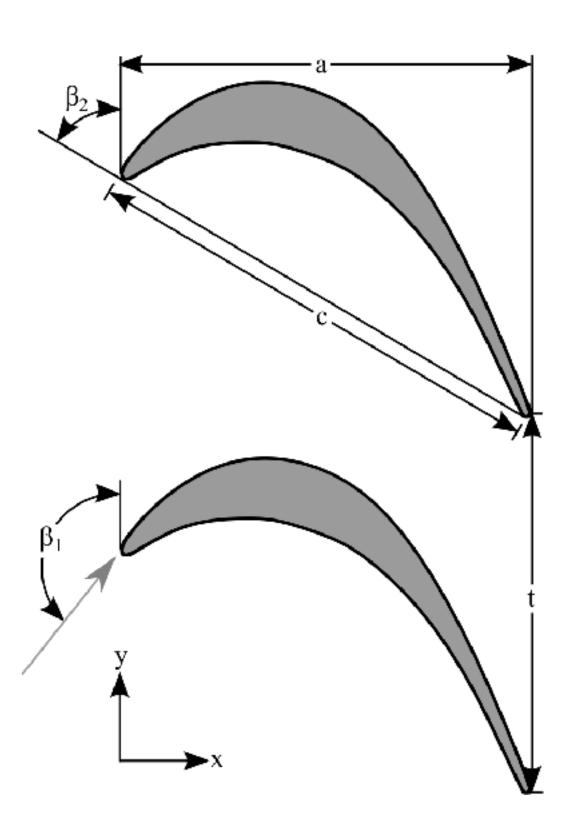
• Time-averaged lift and drag coefficients

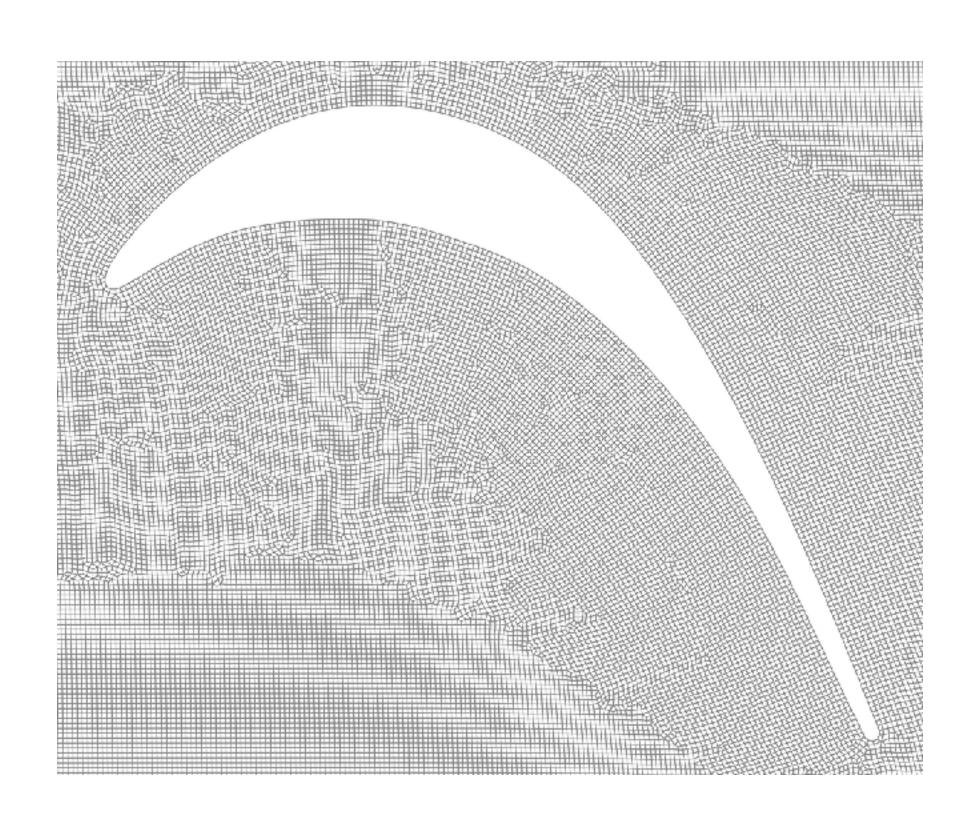


PyFR: T106D

• T106D low pressure turbine cascade at Re = 80,000 and

Ma = 0.4.



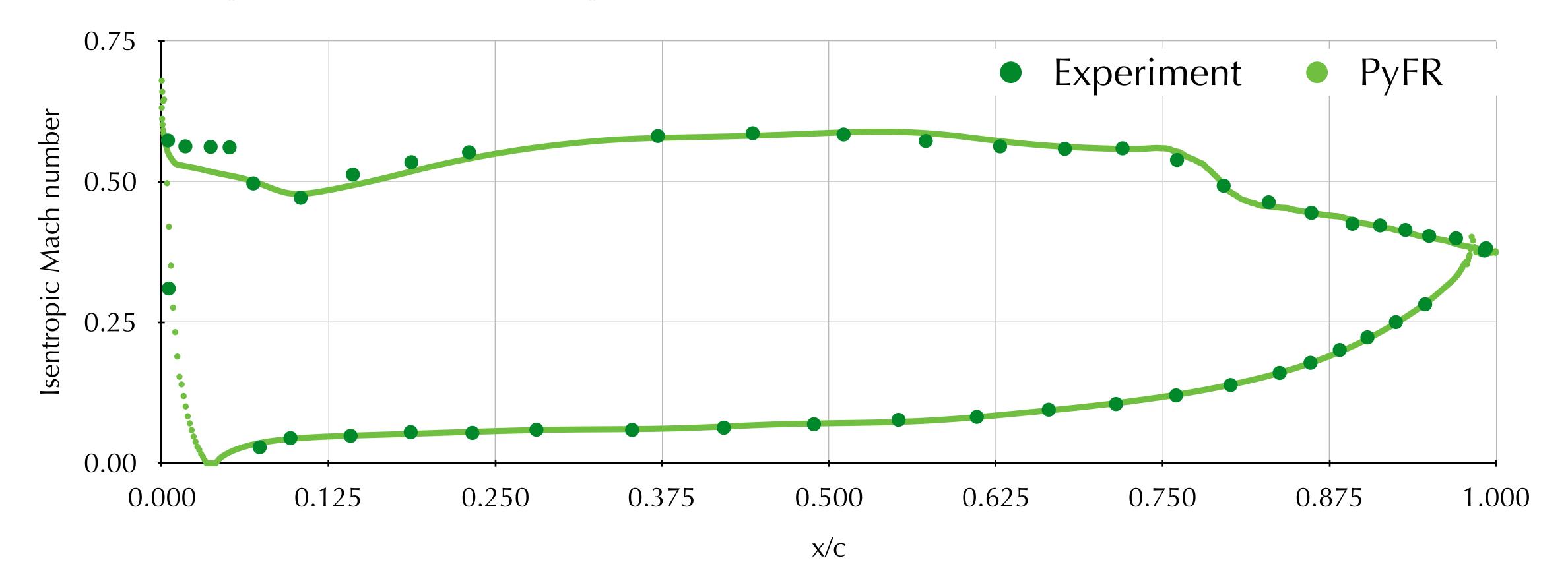


PyFR: T106D

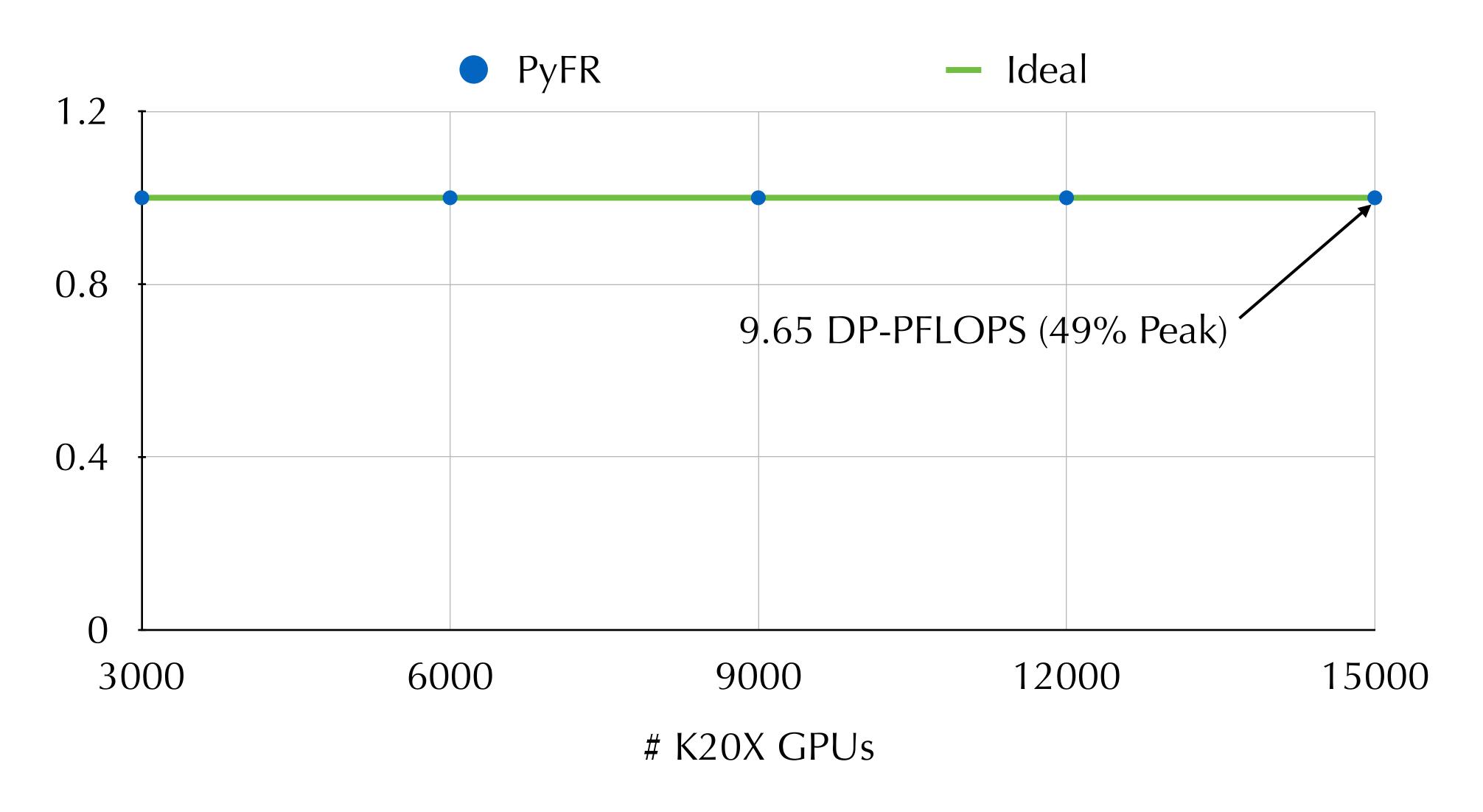


PyFR: T106D

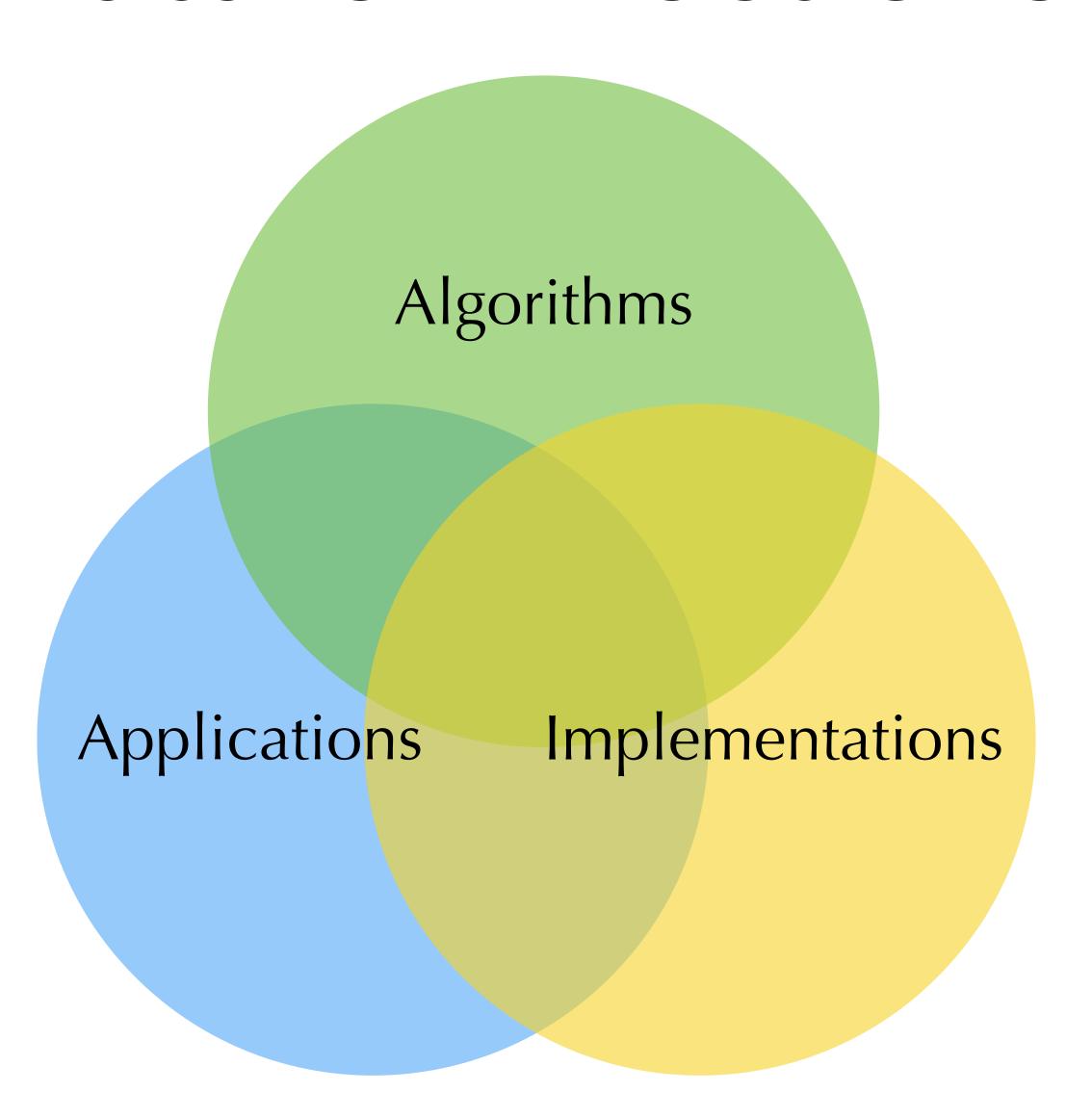
• Comparison with experimental data of P. Stadtmüller et al.

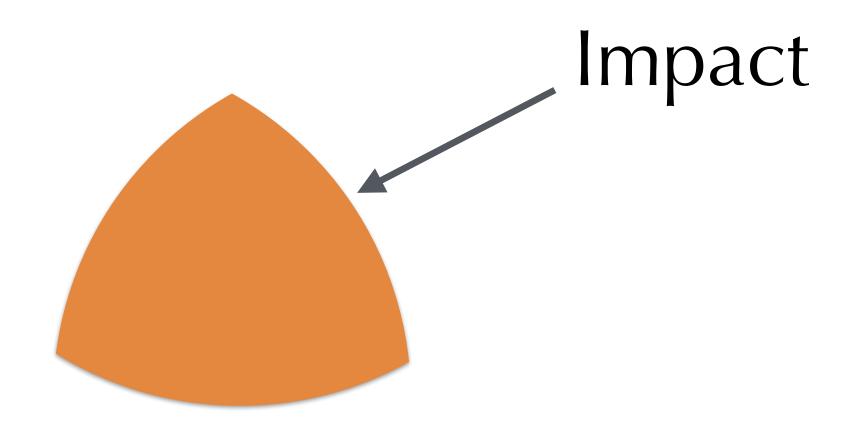


PyFR: Weak Scaling



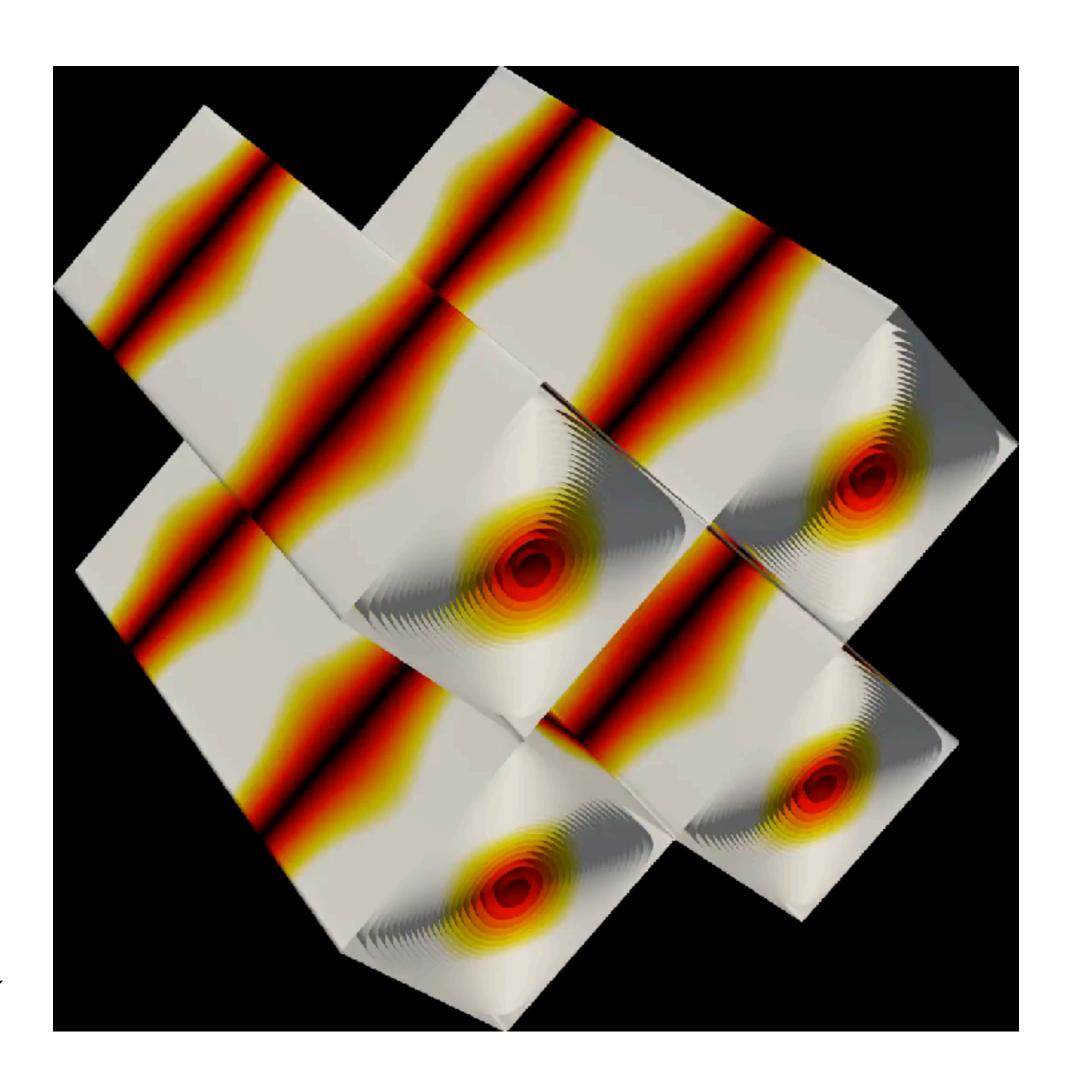
- Numerical methods alone are not enough.
- If we want impact we need to
- ...take ownership of implementing these methods
- ...and applying them to real problems.





- We should thus look to define challenge problems that are relevant to industry.
- Existing test cases are typically far removed from real-world problems.

Evolution of a Taylor—Green vortex



 Real-world problems are large...typically north of one billion DOFs.

- Thus it is vital that we have implementations that are:
- ...efficient on leadership-class DOE systems.
- ...maintainable.

- Developing test cases is also far from trivial.
- Industrial **geometries** and **validation data** are very often **proprietary**.
- Here, collaborations are critical.

- CFD is still a exciting discipline.
- By addressing the challenges herein we can **facilitate a step-change** in several key fields.

- Predicting the future is general ill-advised.
- What follows are the authors' opinions.

- The early development of CFD in the Aerospace Industry was primarily driven by the need to calculate steady transonic flows: this problem is quite well solved.
- CFD has been on a plateau for the past 15 years.
- Advances in numerics and hardware should enable LES for industrial applications in the foreseeable future.

- Industrial LES research should focus on high-order methods for unstructured grids.
- Open issues include: implicit time-stepping, wall and subgrid scale models, curved grid generation, treatment of dynamical grids, fluid structure interaction, and multiphysics.

Eventually DNS may become feasible for high Reynolds number flows.

Hopefully with a smaller power requirement than a wind tunnel.

Acknowledgements

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